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Extension of the Representative Elementary Watershed approach by incorporating energy balance equations

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Abstract

The paper extends the Representative Elementary Watershed (REW) theory for cold regions by extending the energy balance equations to include associated processes and descriptions. A new definition of REW is presented which separates the REW into six surface sub-regions and two subsurface sub-regions. Soil ice, vegetation, vapor, snow and glacier ice are included in the system so that such phenomena as evaporation, transpiration, freezing and thawing can be modeled in a physically reasonable way. The final system of 24 ordinary differential equations (ODEs) can meet the requirement for most hydrological modeling applications, and the formulation procedure is re-arranged so that further inclusion of sub-regions and substances could be done more easily. The number of unknowns is more than the number of equations, which leads to the indeterminate system. Complementary equations are provided based on geometric relationships and constitutive relationships that represent geomorphological and hydrological characteristics of a watershed. Reggiani et al. (1999, 2000, 2001) and Lee et al. (2005b) have previously proposed sets of closure relationships for unknown mass and momentum exchange fluxes. The additional geometric and constitutive relationships required to close the new set of balance equations will be pursued in a subsequent paper.

1 Overview

The current generation of physically-based hydrological models, such as SHE (Abbott et al., 1986a, b), MIKE SHE (Refsgaard and Storm, 1995), IDHM (Beven et al., 1987; Calver and Wood, 1995), and GBHM (Yang et al., 2000, 2002a, 2002b), is based on point scale equations derived from Newtonian mechanics, as first set out by Freeze and Harlan (1969). These physically-based models have distinctive advantages over the so-called conceptual models that are based only on the mass balance principle. The hydrological literature is replete with reviews and discussions of the advantages and limitations of physically-based distributed models (Beven, 1989, 1993, 1996; Grayson et al., 1992; Smith et al., 1994; Woolhiser, 1996; Refsgaard et al., 1996; Singh et al., 2002). The most important limitation is perhaps the mismatch between scale at which the governing equations are applicable and the scale at which models are applied, and the associated difficulties due to the nonlinearity of equations and the heterogeneity of landscape properties. There are two ways to resolve the problem (Beven 1989, 2002). One is to devise effective parameters to account for the heterogeneity while continuing to use the current small-scale governing equations. The other is to devise new equations applicable directly at the spatial scale of a watershed, the scale at which most predictions are required. A number of parameterization schemes have been proposed so far (Viney and Sivapalan, 2004; Robinson and Sivapalan, 1995) to accomplish this. No concerted effort has been made, however, to develop scale adaptable equations which account for the heterogeneity and nonlinearity.

The Representative Elementary Watershed (REW) approach originally outlined by Reggiani et al. (1998, 1999), is an ambitious attempt to invoke mass, momentum, and energy balances and entropy constraints directly at the watershed scale (Beven, 2002). The REW approach treats a watershed as a continuous, open thermodynamic system with discrete sub-watersheds called Representative Elementary Watersheds (REWs), where the REW is deemed as the smallest elementary unit for hydrological modeling. The REW is further divided into several functional sub-regions (in Reggiani et al.'s (1998) formulation, there are five sub-regions, as discussed below in Sect. 2). The division of a watershed into an inter-connected set of discrete REWs is based on the self-similarity nature of the watershed hydrological system. Likewise, the division of the REW into sub-regions is based on the theoretical and practical results of hydrological analysis. REWs and sub-regions are sub-continua of the whole watershed hydrological system. The general conservation laws for mass, momentum, energy, and entropy are then applied to the entire system and to its sub-continua. The resulting ordinary differential equations (ODEs), after averaging over characteristic time and sub-region volume, can then be applied directly at the REW scale.

Many researchers have developed the initial closure relationships required by the REW approach and its numerical models (Reggiani et al., 2000, 2001, 2005; Lee et al., 2005a, 2005b, 2005c; Zhang and Savenije, 2005). The application of these closure relationships to hypothetical, experimental, and natural watersheds shows that the REW approach can indeed simulate and predict watershed hydrological response soundly and reasonably. The REW approach, however, cannot presently take full and comprehensive account of energy processes occurring on the land surface, such as evaporation, transpiration, freezing, and thawing, because of the assumptions used in the original formulation and implementation. These energy processes, which help drive the hydrological cycle, must be elementary components of hydrological models. In order to serve as an alternative blueprint for hydrological modeling, therefore, the REW approach needs to extend its balance equations and constitutive relationships by factoring various additional physical energy processes in a reasonable way.

The purpose of this paper, then, is to re-derive the REW scale balance equations by following Reggiani's procedure, but explicitly including the additional energy processes. We begin with a summary of Reggiani et al.'s REW definition and their REW scale balance equations. We then discuss Reggiani et al.'s definition of REW and present our own definition based on an expanded application of the concept of the REW. After introducing the symbols and notations related to the introduced variables, we use these to describe the geometric, kinetic, and thermodynamic properties of hierarchical continua. We then re-configure the general form of the balance equations for mass, momentum, energy, and entropy at the REW scale by applying the averaging method pioneered by Hassanizadeh and Gray (1979a, 1979b, 1980). To confine the problem to understandable and manageable levels, a series of simplifying assumptions are then presented. Finally, a new set of ordinary differential equations is proposed. In order to facilitate the adoption of the new equations in hydrological modeling practice, the relevant geometric relationships need to be presented and improved. Likewise, the constitutive relationships for the new exchange terms for mass, momentum and energy also need to be devised, and revised. While acknowledging that these are essential, their actual derivation will not be presented here; instead, they will be presented in a subsequent paper.

2 Review of the REW definition and REW scale balance equations for mass and momentum by Reggiani et al. (1998, 1999)

From a hydrological perspective, a watershed and its hierarchical sub-watersheds present self-similar characteristics. We consider a sub-watershed as a fundamental component of hydrological modeling termed the Representative Elementary Watershed. Reggiani et al. (1998, 1999) divide a watershed into REWs, and then further divide each sub-watershed into five sub-regions (see Fig. 1): the saturated zone, the unsaturated zone, the saturated overland flow zone, the concentrated overland flow zone, and the main channel reach. Table 1 shows all the sub-regions in a REW and their respective substances.

Based on the division of catchment into discrete catchment zones (REWs) and sub-regions, Reggiani et al. (1998) derive global balance laws for mass, momentum, energy, and entropy at the spatial scale of REW. After simplification and reduction, a simplified set of REW-scale balance equations of mass and momentum are presented in Eq. (1) to Eq. (11) below. For further detail regarding the meaning of the variables, the reader is referred to Reggiani et al. (1998, 1999, and 2000).

$$\underbrace{\frac{d}{dt}(\varepsilon y^s \omega^s)}_{storage} = \underbrace{e^{so}}_{seepage} + \underbrace{e^{su}}_{exchag.\ with\ unsat.\ zone} + \underbrace{e^{sr}}_{sat.\ zone-river\ exchange} + \underbrace{\sum_l e_l^{sA} + e_{ext}^{sA}}_{exchange\ across\ mantle\ segments} \quad (1)$$

$$\underbrace{\frac{d}{dt}(\varepsilon y^u \omega^u s^u)}_{storage} = \underbrace{e^{uc}}_{infiltration} + \underbrace{e^{us}}_{exchag.\ with\ sat.\ zone} + \underbrace{e_{wg}^{u}}_{evaporation} + \underbrace{\sum_l e_l^{uA} + e_{ext}^{uA}}_{exchange\ across\ mantle\ segments} \quad (2)$$

$$\underbrace{\frac{d}{dt}(y^c\omega^c)}_{storage} = \underbrace{e^{cu}}_{infiltration\ into\ unsat.\ zone} + \underbrace{e^{co}}_{flow\ to\ sat.\ overl.\ flow} + \underbrace{e^{ctop}}_{rainfall\ or\ evaporation} \tag{3}$$

$$\underbrace{\frac{d}{dt}(y^o\omega^o)}_{storage} = \underbrace{e^{or}}_{lat.\ channel\ inflow} + \underbrace{e^{os}}_{seepage} + \underbrace{e^{oc}}_{inflow\ from\ conc.\ overl.\ flow} + \underbrace{e^{otop}}_{rainfall\ or\ evaporation} \tag{4}$$

$$\underbrace{\frac{d}{dt}(m^r\xi^r)}_{storage} = \underbrace{e^{ro}}_{lateral\ inflow} + \underbrace{e^{rs}}_{channel-sat.\ zone\ exch.} + \underbrace{\sum_l e_l^{rA} + e_{ext}^{rA}}_{inflow,\ outflow} + \underbrace{e^{rtop}}_{rainfall\ or\ evaporation} \tag{5}$$

$$\underbrace{\pm\sum_l \boldsymbol{A}_{l,\lambda}^{sA}[-p^s + \rho(\phi_l^{sA} - \phi^s)]}_{inter-REW\ driving\ force} + \underbrace{\pm\boldsymbol{A}_{ext,\lambda}^{sA}[-p^s + \rho(\phi_{ext}^{sA} - \phi^s)]}_{force\ acting\ on\ the\ external\ boundary} + \underbrace{\pm\boldsymbol{A}_{\lambda}^{s\,bot}[-p^s + \rho(\phi^{s\,bot} - \phi^s)]}_{force\ at\ the\ bottom\ boundary}$$

$$= \underbrace{-R^s v_\lambda^s}_{resistance\ to\ flow} \quad ;\lambda = x, y \tag{6}$$

$$\underbrace{\pm\sum_l \boldsymbol{A}_{l,\lambda}^{uA}[-p^u + \rho(\phi_l^{uA} - \phi^u)]}_{inter-REW\ driving\ force} + \underbrace{\pm\boldsymbol{A}_{ext,\lambda}^{uA}[-p^u + \rho(\phi_{ext}^{uA} - \phi^u)]}_{force\ acting\ on\ the\ external\ boundary} = \underbrace{-R^u v_\lambda^u}_{resistance\ to\ flow} \quad ;\lambda = x, y \tag{7}$$

$$\underbrace{[-p^u - \rho(\phi^{uc} - \phi^u)]\varepsilon\omega^u}_{force\ top} - \underbrace{\rho\varepsilon s^u y^u \omega^u g}_{gravity} = \underbrace{-R^u v_z^u}_{resistance\ force} \tag{8}$$

$$\underbrace{(\rho y^c\omega^c)\frac{dv^c}{dt}}_{inertial\ term} - \underbrace{\rho y^c\omega^c g\sin\gamma^c}_{gravity} = -\underbrace{U^c v^c|v^c|}_{resistance\ to\ flow} \tag{9}$$

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$$\underbrace{(\rho y^o \omega^o)\frac{dv^o}{dt}}_{inertial\ term} - \underbrace{\rho y^o \omega^o g \sin\gamma^o}_{gravity} = - \underbrace{U^o v^o |v^o|}_{resistance\ to\ flow} \tag{10}$$

$$\underbrace{(\rho m^r \xi^r)\frac{dv^r}{dt}}_{inertial\ term} = \underbrace{\rho g m^r \xi^r \sin\gamma^r}_{gravitional\ force} - \underbrace{U^r v^r |v^r|}_{Chezy\ resistance}$$
$$+ \underbrace{\pm \sum_l \boldsymbol{A}_l^{rA} \cos\delta_l[-p^r + \rho(\phi_l^{rA} - \phi^r)]}_{pressure\ forces\ exchanged\ among\ REWs} + \underbrace{\boldsymbol{A}_{ext}^{rA}[-p^r + \rho(\phi_{ext}^{rA} - \phi^r)]}_{pressure\ force\ at\ watershed\ outlet} \tag{11}$$

To summarize, Eq. (1) to Eq. (5) represent, respectively, mass balance of the five sub-regions. Eq. (6) to Eq. (11) represent, respectively, momentum balance of the saturated zone in the horizontal direction, unsaturated zone in the horizontal direction, unsaturated zone in the vertical direction, concentrated overland flow zone, saturated overland flow zone, and the channel reach.

In Reggiani et al.'s formulation, energy balance equations are considered as identical equations and omitted due to their isothermal assumption (Reggiani et al., 1999). Vegetation, snow, and ice are not included in the approach so that evapotranspiration, freezing, thawing, and melting cannot be simulated in a physically reasonable way, and thus precludes the application of the REW approach and associated models in cold regions. Generalizing the REW theory to reflect processes in cold regions, through an explicit treatment of energy balance equations, is the subject matter of this paper.

3 Redefinition of Representative Elementary Watershed

We have reviewed Reggiani et al.'s definition of REW in Sect. 2 above. As an initial attempt, their definition exhibits the following limitations:

(1) Phases such as soil matrix, gas, and water are included in the definition, but phases such as ice and snow are excluded. Hydrological phenomena such as accumulation and depletion of glacier and snow pack and freezing and thawing of the soil ice are, therefore, excluded from consideration.

(2) Vegetation is not explicitly considered. Therefore, evapotranspiration cannot be simulated in a physically reasonable way. Evaporation and transpiration cannot be partitioned, either. In Reggiani et al.'s formulation, evapotranspiration is deemed a phase transition from liquid to vapor which occurs within the unsaturated zone, i.e., the soil. This assumption is not physically-based since transpiration as a vaporization process occurs across leaf stomas, and evaporation occurs mainly on the land surface (i.e., soil surface and water surface, and also intercepted water on wet leaf surfaces). The vaporization of water within the soil is small compared with evapotranspiration (Adrie, 1999) and can, therefore, be omitted.

(3) Separation of saturated overland flow from concentrated overland flow is done conceptually rather than in any physically based way. The runoff generated from hillslope can be divided into infiltration excess flow (Hortonian overland flow, also known as concentrated overland flow in Reggiani et al.'s formulation) and saturation excess flow (saturated overland flow) (Dunne, 1975). Infiltration excess runoff occurs when the rainfall intensity is greater than the infiltration capacity of the soil, and saturation excess runoff occurs when the water content of top soil reaches saturation by a rise of water table from below. This distinction, however, only makes conceptual sense. As mentioned, where the saturation excess runoff occurs the water table reaches the land surface which can then be seen as the interface between the water body and the atmosphere. The water body is impermeable (zero infiltration capacity), so the saturation excess runoff can be generated so far as rainfall is greater than evaporation. From this point of view, the saturation excess runoff can be seen as a subset of infiltration excess runoff. Furthermore, the pattern of runoff generation can vary with the intensity and du-

ration of rainfall on a specific location in a watershed. The case is true also for subsurface flow, groundwater flow, and other runoff generation mechanisms (Rui, 2004). Generally, different runoff generation mechanisms have no clear intrinsic distinction. Different types of runoff generation may occur on the interface formed by media with different infiltration capacities, and the infiltration capacity of the upper medium must be higher than that of the lower medium. Runoff is generated when the intensity of water supply to the interface (cannot exceed the infiltration capacity of the upper medium) exceeds the infiltration capacity of the lower medium. Therefore, from this perspective, it is unnecessary to separate the saturation excess runoff from the infiltration excess runoff any more. For these reasons, these concepts are abandoned in the current generation of physically-based models (Freeze and Harlan, 1969), and the surface runoff generation is the result of differential soil water movement. In the REW approach, which is physically based, these concepts should be also abandoned altogether.

(4) That the sub-REW-scale network of channels, rills and gullies is included in the concentrated overland flow zone is somewhat ambiguous. The sub-REW-scale network of channels, rills, gullies, as well as lakes, reservoirs, etc. are water bodies, and their role in hydrological processes is distinct from that of the land surface. The sub-stream network can serve as not only runoff generation areas but also runoff routing pathways, and the latter is more important. We cannot represent the sub-REW-scale runoff routing function physically if the sub-stream network is embedded in the other sub-regions.

We re-define the REW as follows in order to remedy the deficiencies identified above. First, the hydrological processes occurring on the land surface and in the subsurface of a watershed exhibit prominent differences. Land surface receives, reallocates, and transfers the precipitation by means of the hillslope and channel network, which differs obviously from actions occurring beneath the land surface. The flow time scales of the surface water and subsurface water differ in magnitude (Reggiani et al., 1998; Dunne, 1978). Water movement on the land surface can be more easily observed than that beneath the surface. The surface layer, therefore, is separated from the subsurface layer in the new REW formulation.

Second, for the subsurface layer, similar to Reggiani et al.'s definition, the REW is divided into a saturated zone and an unsaturated zone with the water table as the interface. The section below the water table is the saturated zone, while the section above the water table (and beneath the land surface) is the unsaturated zone. For consideration of soil freezing and thawing, the ice phase is included in both the saturated and unsaturated zones, in addition to soil matrix, liquid water, and gas.

Third, for the surface layer, the most striking feature observed is the inter-connected system of hillslopes organized around the river network. From the hydrological point of view, hillslopes and the channel network are two fundamental components of a watershed. Therefore, the surface layer is divided into two sections – hillslope and stream network.

Fourth, a stream network can be further divided into the main channel reach and the sub-stream network. We incorporate lakes, reservoirs, rills, and gullies into the sub-stream network in order to maintain scale invariability in the REW structure.

Finally, hillslopes, which are the primary regions for runoff generation and water dissipation, can be divided into four zones: bare soil, vegetated, snow covered, and glacier covered.

In summary, we defined two sub-regions in the subsurface layer and six sub-regions in the surface layer of a REW (see Table 2 and Fig. 2). Bare soil, vegetation, snow, and glacier represent four fundamental land surface types. By choosing a proper spatial scale according to data availability and the simulation objective, a watershed can be divided into discrete REWs with unique soil types, vegetation categories, snow and glacier cover characteristics, in a similar way that the SWAT model defines Hydrological Response Units (Arnold et al., 1998; Srinivasan et al., 1998). There is no doubt that some special surface sub-regions will be needed in special situations. The six defined types of surface sub-regions, however, should be sufficient for most watershed scale hydrological modeling. New sub-regions can easily be added to the existing REW system without violating the general form of balance equations derived below according to our rules. Certainly, new sub-regions will introduce new exchange terms of mass, momentum, and energy. These will require the specification of additional geometric and constitutive relationships for the closure and determinacy of the balance equations.

On the spatial side, the six surface sub-regions constitute a complete cover of the land surface in the horizontal direction (see Fig. 2). In the vertical direction, we assume the four sub-regions of bare soil, vegetated, snow covered, and glacier covered zones lie above the unsaturated zone. The other two surface sub-regions, i.e., main channel reach and sub-stream network zone, may lie above either the saturated or the unsaturated zone relative to their relationship to the water table.

In order to consider evaporation and transpiration separately, the vapor phase is included in all the surface sub-regions. For subsurface sub-regions, the unsaturated zone also has a vapor phase which coexists with air in the soil pores. We define the mixture of water vapor and air, therefore, as the gaseous phase for the unsaturated zone (and snow covered zone, as detailed below). No evaporation occurs in the subsurface sub-regions, including the unsaturated zone (see discussion about Reggiani et al.'s definition at the beginning of this section). Whereas the vapor phase is included in each surface sub-region, it cannot be stored. The vapor phase disperses into the atmosphere immediately after its formation due to the phase transition from liquid water, snow or ice to vapor. The snow covered zone is an exception to this rule. It includes snow, liquid water, and gas and in this way it is similar to the porous media. The snow covered zone can contain liquid water to a certain degree as saturation content in the soil. The water storage in bare soil zone represents depression storage, the water storage in the vegetated zone represents canopy interception and also depression storage, whereas water cannot be stored in the glacier covered zone. In each case, the liquid water gathered from rainfall in the surface sub-regions, or transferred from ice in the glacier covered zone, or transferred from snow in the snow covered zone, flows into the sub-stream network.

Surface runoff can be generated only when the intensity of rainfall exceeds the infiltration capacity for each surface sub-region. Subsurface flow can be generated when soil is heterogeneous in the unsaturated zone. For example, if the unsaturated zone is divided into two layers and the infiltration capacity of the top layer is greater than that of the lower layer, subsurface flow can generated on the interface between the top and the lower layer. In Reggiani et al.'s definition, and even in our new definition of REW, this heterogeneity is excluded explicitly in order to avoid over-complexity, and the subsurface flow and associated preferred flow are embedded in the mass exchange terms between the unsaturated zone and the neighboring REW or the external world, and accounted for by the corresponding constitutive relationships. For further detailed description of subsurface flow physically, one could separate the unsaturated zone into different layers; this is left for further research.

For details about materials associated with every sub-region, see Table 3, and for a summary of all the different materials involved in the REW, see Table 4.

The sub-region zones are further described below.

Saturated zone: The physical upper boundary of the saturated zone is marked by the water table. The lower boundary is marked either by a limit depth reaching into the groundwater reservoir or by the presence of an impermeable stratum. In the near-channel regions where the water table reaches the soil surface, the physical upper boundary of the saturated zone is coincident with the land surface. These areas can be considered part of the sub-stream network. Laterally the saturated and unsaturated zones are isolated by the mantle surface from the neighboring REWs or by the external watershed boundary.

The materials contained within the saturated zone are the soil matrix, liquid water, and ice. The soil matrix and ice form the skeleton for water movement and phase transition between liquid water and ice may result from natural energy processes.

Unsaturated zone: The physical upper boundary of the unsaturated zone is marked by the land surface. The lower boundary is marked by the water table. The materials contained within the unsaturated zone are the soil matrix, liquid water, gas, and ice.

Evaporation within the soil pores is little and omitted. Mass exchange terms include infiltration from the land surface, recharge into or capillary from the saturated zone, thawing or freezing, and lateral inflow/outflow through the mantle surface.

The location and area/volume of the unsaturated zone depend on the water table fluctuation, geomorphology, and hydrogeologic characteristics. We can estimate the dynamic spatial extent (area/volume) of the unsaturated zone with the help of a digital elevation model (DEM) and Geographic Information System (GIS) software, provided that the location of the dynamic water table could be specified or estimated.

Main channel reach: The main channel reach receives water from the sub-stream network and transfers it towards the watershed outlet. It also exchanges water with the saturated zone. Of all the surface sub-regions, this is the only zone which can exchange water, momentum with the neighboring REWs or the external world. The water course of main channel reach can be determined either by field observation or by DEM analysis. The materials contained within the main channel reach are water and vapor.

Sub-stream network zone: The sub-stream network zone is the areal volume occupied by lakes, reservoirs, and the sub-REW-scale network of channels, rills, gullies, and ephemeral streams. It gathers water from the hillslopes and transfers it into the main channel reach. Its storage capacity and flow velocity are of importance for sub-REW-scale runoff routing. The substances contained within the sub-stream network zone are water and vapor.

Vegetated zone: The vegetated zone is the volume occupied by vegetation which intercepts precipitation, extracts water from the unsaturated zone through the roots, and evaporates it into the atmosphere in the form of transpiration. The water storage of this zone represents canopy interception storage and depression storage. The projected area of this zone changes with the calendar and the cultivation season. The materials contained in the vegetation covered zone are vegetation, water, and vapor.

Snow covered zone: The snow covered zone is the volume of snow pack which plays an important role in hydrology and the energy cycle. The location of the snow covered zone can be determined by field or remote observation. Its area and depth are key factors for hydrological modeling in cold regions. They cannot be easily recognized and much literature can be found about their measurement and modeling. The materials contained in the snow covered zone are snow, water, and gas.

Glacier covered zone: The glacier covered zone is the volume occupied by glacier ice which location is always fixed. The materials contained in this zone are ice, liquid water, and vapor. On the hydrological time scale, the glacier covered area can be seen as invariant.

Bare soil zone: The bare soil zone is the volume occupied neither by vegetation, nor by snow, nor by glacier, nor by the sub-stream network, nor by the main channel reach. The water storage of this zone represents only the depression storage. The horizontal projected area varies with the areas of the other surface sub-regions. The substances contained in this zone are bare soil, liquid water, and vapor.

4 Geometric, kinetic, and thermodynamic properties of hierarchical continua

In the REW approach, the entire watershed system is constituted by a finite number M of discrete REWs. Each REW is then divided into two subsurface sub-regions and six surface sub-regions. Several materials are included within each sub-region. In terms of thermodynamics, the watershed system is composed of three hierarchical subsystems.

(1) REW level: every discrete REW is treated as a subsystem of the entire watershed system. There are M discrete REW level subsystems in a watershed made up of M REWs;

(2) Sub-region level: every sub-region in a REW is treated as a subsystem of the REW level thermodynamic system. There are eight sub-region level subsystems in one REW level system;

(3) Phase level: every type of substance in a sub-region is treated as a subsystem of a sub-region level thermodynamic system. The number of subsystems included

in a sub-region level system can be counted from Table 3, and there are in all 23 phase level subsystems in one REW level system.

We can thus regard the watershed, the REWs, the sub-regions, and the phases as hierarchical continua from a continuous medium mechanics perspective. Before applying conservation laws for subsystems or the continua as defined above, we will describe in turn the geometric, kinetic, and thermodynamic properties at the REW level, sub-region level, and phase level.

4.1 Geometric description of the REW level continuum

The number of discrete REWs in a watershed is denoted by M. The kth REW is marked by $B(K), K \in \{e|e=1..M\}$, where B indicates the body of a continuum. The number of REWs neighboring $B(K)$ is denoted by N_K. The space occupied by all the materials contained within $B(K)$ is denoted by $V(K)$ where $V(K)$ is a prismatic volume (for details the reader should refer to Reggiani et al., 1998).

The surface of the prism is recorded as $S(K)$ which includes side, top, and bottom surfaces.

(1) Side surfaces: the side surface of $B(K)$ can be divided into a series of segments: the interfaces with $B(L)$ $(L=1...N_K)$, or the interfaces with the external world (in case $B(K)$ is located on the boundaries of the watershed). The segment formed by the interfaces between $B(K)$ and $B(L)$ $(L=1...N_K)$ is denoted by $S^{,L}(K)$. The segment formed by the interfaces between $B(K)$ and the external world is denoted by $S^{,EXT}(K)$.

(2) Top surface: the top surface of $B(K)$ formed by the land surface covering $B(K)$ is an irregular curved surface which is denoted by $S^{,T}(K)$. The projection of $S^{,T}(K)$ onto the horizontal plane is denoted by $\sum(K)$, and the contour of $S^{,T}(K)$ is denoted by $C(K)$. $C(K)$ is coincident with the natural boundary of the REW (i.e.

ridges and divides). The nadir of $C(K)$ is the watershed outlet and is denoted by $P^{o}(K)$.

(3) Bottom surface: the bottom surface of $B(K)$, denoted by $S^{,B}(K)$, is the impermeable strata or a hypothetical plane at a given depth reaching into the groundwater reservoir or the combination of the two. When it is the impermeable strata, the bottom surface is an irregular curved surface with regard to the geological characteristics.

4.2 Geometric description of the sub-region level continuum

The sub-region level continua divided from $B(K)$ and the phase level continua included in a sub-region are denoted by $B^{j}(K)$ and $B^{j}_{\alpha}(K)$ respectively, where $j \in \{e \,|\, e = u, s, r, t, b, v, n, g\}$, $\alpha \in \{\zeta \,|\, \zeta = m, l, a, p, i, n, v\}$ (see Table 3). The volumes occupied by $B^{j}(K)$, $B^{j}_{\alpha}(K)$ are denoted by $V^{j}(K)$, $V^{j}_{\alpha}(K)$, respectively. $B^{s}(K)$ (the saturated zone) and $B^{u}(K)$ (the unsaturated zone) occupy a 3-D space, while $B^{r}(K)$ (the main channel reach) is linear, while the other zones are planar.

$B^{j}(K)$ exchanges mass, momentum, and energy with environment through its interface $S^{j}(K)$, which can be divided into the following components:

(1) Interfaces between $B^{j}(K)$ and the external world, which is denoted by $S^{jEXT}(K)$. If $B(K)$ is located within the watershed, or located on the boundaries while $B^{j}(K)$ is located within the watershed, then $S^{jEXT}(K) = 0$.

(2) Interfaces between $B^{j}(K)$ and $B(L)$ $(L = 1 \ldots N_{K})$, which is denoted by $S^{jL}(K)$. If $B^{j}(K)$ is located within $B(K)$, then $S^{jL}(K) = 0$.

(3) Interfaces between $B^{j}(K)$ and the atmosphere on the top, which is denoted by $S^{jT}(K)$. This surface corresponds to that part of the land surface covering the REW for surface sub-regions and its area is zero for subsurface sub-regions.

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(4) Interfaces between $B^j(K)$ and the impermeable strata or groundwater reservoir at the bottom, which is denoted by $S^{jB}(K)$.

(5) Interfaces between $B^j(K)$ and the other sub-regions within the same REW, $B^i(K)$ $(i \neq j)$, which is denoted by $S^{ji}(K), (i \neq j)$.

In our derivation, we use $d\mathbf{S}$ to denote the differential area vector of the surface. For the surfaces discussed above, the corresponding differential area vector symbols, $d\mathbf{S}^{jEXT}(K)$, $d\mathbf{S}^{jL}(K)$, $d\mathbf{S}^{jT}(K)$, $d\mathbf{S}^{jB}(K)$, and $d\mathbf{S}^{ji}(K)$, are defined. These differential vectors point to the side indicated by the second superscript from the side indicated by the first superscript along the normal direction of the differential area, and the following equations hold

$$\left.\begin{aligned} S^{ji} &= S^{ij} \\ d\mathbf{S}^{ji} &= -d\mathbf{S}^{ij} \end{aligned}\right\} j \neq i \,. \tag{12}$$

We also define the area vector for interface S^{jP} as

$$\mathbf{S}^{jP} = \int_{S^{jP}} d\mathbf{S}^{jP}, P = EXT, L, T, B, i, L = 1..N_k, i \neq j \,. \tag{13}$$

4.3 Definition of the time-averaged REW-scale quantities

In watershed hydrological processes, geometric, kinetic, and thermodynamic quantities for the differential volume in the continua defined above change constantly. To formulate the balance equations at the macroscale of both time and space, we average the corresponding quantities in time and space. Here some definitions of averaged quantities are presented for later use.

In the following sections, the identifier of individual REW, K, is omitted in the interest of brevity unless confusion arises in which case it is included.

Definition 1: The fraction of time-averaged horizontal projected area of B^j in Σ, $j \neq r$

$$\omega^j = \frac{1}{2\Delta t \Sigma} \int_{t-\Delta t}^{t+\Delta t} \Sigma^j(\tau)\, d\tau,\ j \neq r, \tag{14}$$

where $2\Delta t$ is the time interval, Σ is the horizontal projected area of $B(K)$, Σ^j is the horizontal projected area of B^j.

Definition 2: The time-averaged thickness of B^j, $j \neq r$

$$y^j = \frac{1}{2\Delta t \omega^j \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_{V^j} dV\, d\tau,\ j \neq r \tag{15}$$

Definition 3: The time-averaged volume of B_α^j relative to V^j, $j \neq r$

$$\varepsilon_\alpha^j = \frac{1}{2\Delta t y^j \omega^j \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_{V^j} \gamma_a^j dV\, d\tau,\ j \neq r \tag{16}$$

where γ_a^j is the phase distribution function on α phase in j sub-region, see Definition 10 below for detail. For the saturated and unsaturated zone, ε_l^j (j=u, s) indicates water content.

Definition 4: The time-averaged density of B_α^j, $j \neq r$

$$\overline{\rho_\alpha^j} = \frac{1}{2\Delta t \varepsilon_\alpha^j y^j \omega^j \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_{V^j} \rho_\alpha^j \gamma_a^j dV\, d\tau,\ j \neq r \tag{17}$$

where ρ_α^j is the density of α phase at the differential volume dV in V_α^j space.

Definition 5: The time-averaged physical quantity $\boldsymbol{\phi}$ possessed by B_α^j relative to the mass of B_α^j, $j \neq r$

$$\overline{\psi_\alpha^j} = \frac{1}{2\Delta t \overline{\rho_\alpha^j} \varepsilon_\alpha^j y^j \omega^j \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_{V^j} \rho_\alpha^j \psi_\alpha^j \gamma_a^j dV\, d\tau,\ j \neq r \tag{18}$$

Definition 6: The time-averaged lenght of the main channel reach relative to Σ

$$\xi^r = \frac{1}{2\Delta t \Sigma} \int_{t+\Delta t}^{t-\Delta t} L^r d\tau \,, \tag{19}$$

where L^r is the instantaneous length of the main channel reach. It is constant in most cases, and ξ^r is, therefore, constant too.

Definition 7: The time-averaged cross section area of the main channel reach

$$m^r = \frac{1}{2\Delta t \xi^r \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_{V^r} dV d\tau \tag{20}$$

Definition 8: The time-averaged density $\overline{\rho_\alpha^r}$ of B_α^r

$$\overline{\rho_\alpha^r} = \frac{1}{2\Delta t m^r \xi^j \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_{V^r} \rho_\alpha^r \gamma_a^r dV d\tau \,, \tag{21}$$

where ρ_α^r is the density of α phase at the differential volume dV in V_α^r space.

Definition 9: The time-averaged physical quantity $\boldsymbol{\phi}$ possessed by B_α^j relative to the mass of B_α^j, $j \neq r$

$$\overline{\psi_\alpha^r} = \frac{1}{2\Delta t \overline{\rho_\alpha^r} m^r \xi^r \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_{V^r} \rho_\alpha^r \psi_a^r \gamma_a^r dV d\tau \,. \tag{22}$$

4.4 Geometric description of the phase level continuum

We introduce the definition of the phase distribution function in order to define physical quantities for the phase level continuum conveniently.

$$\gamma_\alpha^j(dV) = \begin{cases} 1, & dV \in V_\alpha^j \\ 0, & dV \notin V_\alpha^j \end{cases} \tag{23}$$

The physical quantities defined in V_α^j space can be alternatively defined in V^j space with the help of the phase distribution function. This is also true for the physical quantity defined over the interface S_α^j. Therefore, through the use of the phase distribution function, we can omit the definitions of V_α^j and S_α^j, and focus on the phase interfaces between B_α^j and B_β^j ($\beta \neq \alpha$) within one sub-region, which is denoted by $S_{\alpha\beta}^j$, $\beta \neq \alpha$. Similarly, the symbol $d\boldsymbol{S}_{\alpha\beta}^j$ is used for indicating the differential area vector of interface $S_{\alpha\beta}^j$, $\beta \neq \alpha$. It points to β phase from a phase along the normal direction of the differential area, and the following equations denote if:

$$S_{\alpha\beta}^j = S_{\beta\alpha}^j \qquad d\boldsymbol{S}_{\alpha\beta}^j = -d\boldsymbol{S}_{\beta\alpha}^j \qquad \beta \neq \alpha\,. \tag{24}$$

We also define the area vector of interface $S_{\alpha\beta}^j$, $\beta \neq \alpha$ as

$$\boldsymbol{S}_{a\beta}^j = \int_{S_{\alpha\beta}^j} d\boldsymbol{S}_{a\beta}^j, \beta \neq \alpha \tag{25}$$

4.5 REW-scale mass exchange terms through interfaces

Mass exchange terms through interfaces are the most important variables in a hydrological system. Here we define the time-averaged values of various REW-scale mass exchange terms relative to Σ for later use.

Definition 11: The net flux of α phase through S^{jP}

$$e_\alpha^{jP} = \frac{1}{2\Delta t \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_{S^{jP}} \rho_\alpha^j \left(\boldsymbol{w}_\alpha^{jP} - \boldsymbol{v}_\alpha^j\right) \cdot \gamma_a^j d\boldsymbol{A} d\tau, P{=}EXT, L, T, B, i, L{=}1..N_K, i \neq j\,, \tag{26}$$

where $\boldsymbol{v}^j_\alpha$ is the velocity of the continuum B^j_α, $\boldsymbol{w}^{jP}_\alpha$ is the velocity of the interface S^{jP}_α.
Definition 12: The phase transition rate between α phase and β phase

$$e^j_{\alpha\beta} = \frac{1}{2\Delta t \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_{S^j_{\alpha\beta}} \rho^j_\alpha \left(\boldsymbol{w}^j_{\alpha\beta} - \boldsymbol{v}^j_\alpha \right) \cdot \gamma^j_a d\boldsymbol{A} d\tau \quad (27)$$

5 General form of the conservation laws and their averaging

5.1 General form of the conservation laws

In the REW approach, the derivations of the balance equations are based on the global conservation laws written in term of a generic thermodynamic property ψ. The averaging method developed by Hassanizadeh et al. (1979a, 1979b, 1980, 1986a, 1986b) and pioneered by Reggiani et al. (1998, 1999) is then applied.

Suppose a control volume V^* and its boundary surface is $A^*=\partial V^*$. At a specific time, the substances contained in V^* form a continuum B. For a conserved physical quantity ψ, the Euler description of its global generic conservation law is:

$$\frac{\partial}{\partial t} \int_{V^*} \rho\psi dV + \int_{A^*} \rho\psi (\boldsymbol{v} - \boldsymbol{w}) \cdot d\boldsymbol{A} - \int_{A^*} \boldsymbol{i} \cdot d\boldsymbol{A} - \int_{V^*} (\rho f + G)\, dV = 0\,, \quad (28)$$

where ρ is the mass density of the continuum, dV is the differential volume, dA is the differential area of the interface, $d\boldsymbol{A}$ is the differential area vector of the interface whose value is dA, direction is the normal direction pointing outward, $\boldsymbol{v}$ is the velocity of a continuum, $\boldsymbol{w}$ is the velocity of a continuum interface, ψ is the specific physical quantity $\boldsymbol{\phi}$ with mass, $\boldsymbol{i}$ is the diffusion flux, f is the source or sink term per unit mass, G is the source or sink term per unit volume. The quantities $\boldsymbol{i}$, f and G have to be chosen depending on the type of physical quantity $\boldsymbol{\phi}$ that is considered (see Table 5 for detail).

5.2 General form of the time averaged conservation laws on the spatial scale of REW

Applying Eq. (28) to a phase level continuum B_α^j yields

$$\frac{\partial}{\partial t}\int_{V_\alpha^j}\rho_\alpha^j\psi_\alpha^j dV + \sum_{P=EXT,L,T,B,i}^{L=1\ldots N_K,i\neq j}\int_{S^{jP}}\rho_\alpha^j\psi_\alpha^j\left(\boldsymbol{v}_\alpha^j-\boldsymbol{w}_\alpha^{jP}\right)\cdot\gamma_a^j d\boldsymbol{A}+\sum_{\beta\neq\alpha}\int_{S_{\alpha\beta}^j}\rho_\alpha^j\psi_\alpha^j\left(\boldsymbol{v}_\alpha^j-\boldsymbol{w}_{\alpha\beta}^j\right)\cdot d\boldsymbol{A}$$
$$-\sum_{P=EXT,L,T,B,i}^{L=1\ldots N_K,i\neq j}\int_{S^{jP}}\boldsymbol{i}\cdot\gamma_a^j d\boldsymbol{A}-\sum_{\beta\neq\alpha}\int_{S_{\alpha\beta}^j}\boldsymbol{i}\cdot d\boldsymbol{A}-\int_{V_\alpha^j}\left(\rho_\alpha^j f+G\right)dV=0 \quad (29)$$

All the variables are defined based on the differential volume of the continuum or differential area of the interface. In other words, they are all the microscopic quantities which exhibit a mismatch with the macroscopic quantities required for watershed hydrological modeling. An averaging procedure in both time and space is necessary for obtaining balance equations directly at the spatial scale of the REW. This procedure has been pursued in detail in the Appendix. In this section only the final results are presented. All the equations take the general form against a phase level continuum.

General form of mass conservation equation:

$$\frac{d}{dt}\left(\overline{\rho_\alpha^j}\varepsilon_\alpha^j y^j\omega^j\right)=\sum_{P=EXT,L,T,B,i}^{L=1\ldots N_K,i\neq j}e_\alpha^{jP}+\sum_{\beta\neq\alpha}e_{\alpha\beta}^j \quad (30)$$

General form of momentum conservation equation:

$$\left(\overline{\rho_\alpha^j}\varepsilon_\alpha^j y^j\omega^j\right)\frac{d}{dt}\left(\overline{\boldsymbol{v}_\alpha^j}\right)=\overline{\boldsymbol{g}_\alpha^j\rho_\alpha^j}\varepsilon_\alpha^j y^j\omega^j+\sum_{P=EXT,L,T,B,i}^{L=1\ldots N_K,i\neq j}\boldsymbol{T}_\alpha^{jP}+\sum_{\beta\neq\alpha}\boldsymbol{T}_{\alpha\beta}^j, \quad (31)$$

where the term on the l.h.s. is the inertial term, the first term on the r.h.s. is the weight of water. The remaining terms on the r.h.s. represent the various forces acting on the mantle segments in common with the external watershed boundary, with the neighboring REWs, top interface, bottom interface, interfaces between j sub-region and neighboring sub-regions, and the interfaces between the α phase and the remaining phases, $\overline{\boldsymbol{v}_\alpha^j}$ is the velocity vector of the α phase averaged over the j sub-region, and $\overline{\boldsymbol{g}_\alpha^j}$ is the averaged gravity vector.

General form of heat balance equation:

In Appendix A we present the conservation equation for mechanical energy and internal energy. We also derive the heat balance equation, with the additional terms due to velocity and internal energy fluctuation being ignored. The following heat balance equation is used in hydrological modeling:

$$\left(\varepsilon_\alpha^j y^j \omega^j c_\alpha^j\right) \frac{d\overline{\theta_\alpha^j}}{dt} = \overline{h_\alpha^j \rho_\alpha^j} \varepsilon_\alpha^j y^j \omega^j + \sum_{P=EXT,L,T,B,i}^{L=1\ldots N_K, i\neq j} Q_\alpha^{jP} + \sum_{\beta\neq\alpha} Q_{\alpha\beta}^j, \tag{32}$$

where one the l.h.s. the term represents the derivation of heat storage of α phase in j zone due to the variation of the temperature, on the r.h.s. the first term accounts for heat generation rate of α phase in j zone, the second term represents heat transfer rate from j zone to its environment, and the third term accounts for the heat transfer rate from the α phase to the remaining phases within the j zone, c_α^j is the specific heat capacity at a constant volume of α phase, $\overline{\theta_a^j}$ is the temperature of α phase averaged over V_α^j, $\overline{h_a^j}$ is heat generation rate per unit mass in V_α^j, Q_α^{jP} is the rate of heat transferred from P zone to j zone, and $Q_{\alpha\beta}^j$ is the rate of heat transferred from β phase to α phase within the j zone.

General form of entropy balance equation:

$$\left(\overline{\rho_\alpha^j}\varepsilon_\alpha^j y^j \omega^j\right) \frac{d\overline{\eta_\alpha^j}}{dt} = \overline{b_\alpha^j \rho_\alpha^j}\varepsilon_\alpha^j y^j \omega^j + \overline{L_\alpha^j}\varepsilon_\alpha^j y^j \omega^j + \sum_{P=EXT,L,T,B,i}^{L=1\ldots N_K, i\neq j} F_\alpha^{jP} + \sum_{\beta\neq\alpha} F_{\alpha\beta}^j, \tag{33}$$

where on the l.h.s. the term accounts for the derivation of entropy storage, on the r.h.s. the first term represents the supply rate of entropy from the external world, the second term is the internal entropy production rate within the subsystem, and the remaining terms are the various exchange terms across interfaces with mantle segments in common with the external watershed boundary, with the neighboring REWs, top interface, bottom interface, interfaces between j sub-region and neighboring sub-regions, and interfaces between α phase and the remaining phases.

6 Simplification of the equation sets

In previous sections, we have obtained the general form of the time-averaged conservation equations for mass, momentum, energy, and entropy. In this section, we make a series of assumptions to keep the problem clearer and manageable, while meeting the requirements of hydrological modeling at the watershed scale. Then the interfaces across which the physical quantities such as mass, momentum, energy, and entropy exchange are defined according to the assumptions. Finally, the general form of the averaged conservation laws is applied to each phase level continuum and their final balance equations obtained.

6.1 Assumptions for hydrological modeling in the REW approach

- Assumption 1: Evapotranspiration occurs only in the surface sub-regions, and vapor storage capacity and its velocity can be ignored in all sub-continua.
- Assumption 2: Soil matrix is static, rigid, and inertial.

- Assumption 3: Ice is static and rigid.
- Assumption 4: All substances within the same sub-region possess the same temperature, and all surface sub-regions besides snow covered and glacier covered sub-regions possess the same temperature, which is denoted by $\overline{\Theta^{surf}}$. Moreover, heat transfer only occurs in the vertical direction.

In our assumptions, Reggiani et al.'s assumption of a isothermal system is abandoned. This enables the equations developed in this paper to simulate the energy process. Owing to the above assumptions, we can omit the following equations and mass exchange terms in the final results:

1. Balance equations of mass, momentum, and energy for gaseous substances, including gas and vapor;
2. Balance equations of mass, momentum, and energy for soil matrix;
3. Balance equation of momentum for soil ice;
4. Mass exchange terms between sub-regions are non-zero only for the water phase. The exception is the mass exchange term between j sub-region and atmosphere, e_g^{jT}. However, the atmosphere is not a sub-region of the hydrological system but represents its external environment.

6.2 Interfaces in REW approach

Interfaces isolating the watershed, REW, sub-region and phase decide the exchange terms arising in the balance equations. According to the above assumptions, interfaces in the REW approach are summarized in Table 6.

6.3 Balance equations for saturated zone

Substitution of mass, momentum, and energy exchange terms occurring within the saturated zone in Eq. (30), Eq. (31), and Eq. (32) with the help of the above assumptions leads to various conservation equations as follows:

Balance equation of mass for water phase:

$$\frac{d}{dt}\left(\overline{\rho_l^s}\varepsilon_l^s y^s \omega^s\right) = e_l^{sEXT} + \sum_{L=1}^{N_K} e_l^{sL} + e_l^{sB} + e_l^{su} + e_l^{st} + e_l^{sr} + e_{li}^{s} \tag{34}$$

where the l.h.s. term accounts for the rate of change of water storage, the terms on the r.h.s. are various water exchange rate terms with the external world of the watershed, neighboring REWs, groundwater reservoir, unsaturated zone, sub-stream network, main channel reach, and ice phase respectively. In Eq. (34), e_l^{sB} is zero when the bottom is impermeable, e_l^{su} represents water recharge term from the unsaturated zone into the saturated zone when it is positive, and capillary rise term from the saturated zone into the unsaturated zone when it is negative. e_{li}^{s} accounts for ice thawing when it is positive, and water freezing when it is negative. The first two terms on the r.h.s. can be seen as groundwater flow.

Balance equation of mass for ice:

$$\frac{d}{dt}\left(\overline{\rho_i^s}\varepsilon_i^s y^s \omega^s\right) = e_{il}^{s} = -e_{li}^{s} \tag{35}$$

Balance equation of momentum for water:

$$\overline{\rho_l^s}\varepsilon_l^s y^s \omega^s \frac{d}{dt}\overline{\mathbf{v}_l^s} - \overline{\mathbf{g}_l^s \rho_l^s}\varepsilon_l^s y^s \omega^s = \mathbf{T}_l^{sEXT} + \sum_{L=1}^{N_K} \mathbf{T}_l^{sL} + \mathbf{T}_l^{sB} + \mathbf{T}_l^{su} + \mathbf{T}_l^{st} + \mathbf{T}_l^{sr} + \mathbf{T}_{lm}^{s} + \mathbf{T}_{li}^{s} \tag{36}$$

where the terms on the l.h.s. are the inertial term and weight of water, respectively. The r.h.s. terms represent various forces: the total pressure forces acting on the mantle segments in common with the external watershed boundary and neighboring REWs, the forces exchanged with the groundwater reservoir, the forces transmitted to the unsaturated zone across the water table, to the sub-stream network zone across the seepage face, to the main channel reach zone across the seepage face, and the resultant forces exchanged with the soil matrix and the ice on the water-soil matrix and water-ice interfaces, respectively.

Owing to the Assumption 2 and Assumption 3, we can combine ice and the soil matrix together for momentum exchange. Therefore, the momentum terms of $\mathbf{T}^s_{lm}$ and $\mathbf{T}^s_{li}$ can be united into one single term $\mathbf{T}^s_{l(m,i)}$ which is denoted by $\mathbf{T}^s_{lm}$ unless otherwise confusion would arise.

$$\overline{\rho^s_l}\varepsilon^s_l y^s \omega^s \frac{d}{dt}\overline{\mathbf{v}^s_l} - \overline{\mathbf{g}^s_l}\,\overline{\rho^s_l}\varepsilon^s_l y^s \omega^s = \mathbf{T}^{sEXT}_l + \sum_{L=1}^{N_K}\mathbf{T}^{sL}_l + \mathbf{T}^{sB}_l + \mathbf{T}^{su}_l + \mathbf{T}^{st}_l + \mathbf{T}^{sr}_l + \mathbf{T}^s_{lm} \tag{37}$$

Balance equation of heat for water:

$$\varepsilon^s_l y^s \omega^s c^s_l \frac{d}{dt}\overline{\theta^s_l} - \lambda_l l_{il} e^s_{il} = \kappa^{sB}_l Q^{sB} + \kappa^{su}_l Q^{su} + \kappa^{st}_l Q^{st} + \kappa^{sr}_l Q^{sr}\,, \tag{38}$$

where on the l.h.s. the first term represents the rate of change of heat storage due to variation of the temperature, and the second term represents heat of freezing. The terms on the r.h.s. are REW-scale heat exchange terms of water with the groundwater reservoir, the unsaturated zone, the sub-stream network, the main channel reach, respectively, c^s_l is the specific heat capacity of water in the saturated zone at a constant volume, l_{il} is the latent heat of freezing, λ_l is the ratio of freezing heat absorbed by water, κ^{sB}_l is the ratio of the heat exchange term (across interface between saturated zone and groundwater reservoir) absorbed by water, and $\kappa^{su}_l, \kappa^{st}_l, \kappa^{sr}_l$ is the ratio of corresponding heat exchange term similarly absorbed by water.

Balance equation of heat for ice:

$$\varepsilon^s_i y^s \omega^s c^s_i \frac{d}{dt}\overline{\theta^s_i} - \lambda_i l_{il} e^s_{il} = \kappa^{sB}_i Q^{sB} + \kappa^{su}_i Q^{su} + \kappa^{st}_i Q^{st} + \kappa^{sr}_i Q^{sr}\,, \tag{39}$$

where the meaning of symbols is similar to those of Eq. (38), l_{il} is the latent heat of freezing, λ_i is the ratio of freezing heat absorbed by ice, κ_i^{sB} is the ratio of heat exchange term (across interface between saturated zone and groundwater reservoir) absorbed by ice, and $\kappa_i^{su}, \kappa_i^{st}, \kappa_i^{sr}$ is the ratio of corresponding heat exchange term absorbed by ice.

Balance equation of heat for soil matrix:

$$\varepsilon_m^s y^s \omega^s c_m^s \frac{d}{dt}\overline{\theta_m^s} - \lambda_m l_{il} e_{il}^s = \kappa_m^{sB} Q^{sB} + \kappa_m^{su} Q^{su} + \kappa_m^{st} Q^{st} + \kappa_m^{sr} Q^{sr}, \tag{40}$$

where, similar to Eq. (38) and Eq. (39), λ_m is the ratio of freezing heat absorbed by the soil matrix, κ_m^{sB} is the ratio of heat exchange term (across interface between saturated zone and groundwater reservoir) absorbed by the soil matrix, and $\kappa_m^{su}, \kappa_m^{st}, \kappa_m^{sr}$ is the ratio of corresponding heat exchange term absorbed by the soil matrix.

The sum of the fraction of heat exchange terms absorbed by water, ice, and the soil matrix should be one, i.e.

$$\begin{aligned}
&\kappa_l^{sB} + \kappa_i^{sB} + \kappa_m^{sB} = 1 \\
&\kappa_l^{su} + \kappa_i^{su} + \kappa_m^{su} = 1 \\
&\kappa_l^{st} + \kappa_i^{st} + \kappa_m^{st} = 1 \\
&\kappa_l^{sr} + \kappa_i^{sr} + \kappa_m^{sr} = 1 \\
&\lambda_l + \lambda_i + \lambda_m = 1
\end{aligned} \tag{41}$$

The specific heat capacity is an extensive quantity, so the following equation holds

$$\varepsilon_l^s c_l^s + \varepsilon_i^s c_i^s + \varepsilon_m^s c_m^s = c^s \tag{42}$$

According to Assumption 4,

$$\overline{\theta_l^s} = \overline{\theta_i^s} = \overline{\theta_m^s} = \overline{\theta^s}\ . \tag{43}$$

Adding Eq. (38), Eq. (39), Eq. (40) together, and applying Eq. (41), Eq. (42), and Eq. (43), yields the balance equation of heat for the entire saturated zone:

$$y^s \omega^s c^s \frac{d}{dt} \overline{\theta_l^s} - l_{il} e_{il}^s = Q^{sB} + Q^{su} + Q^{st} + Q^{sr} , \tag{44}$$

where on the l.h.s. the first term represents the rate of change of heat storage due to variation of the temperature, and the second term represents the rate of freezing heat. The terms on the r.h.s. are REW-scale heat exchange terms of water with the groundwater reservoir, the unsaturated zone, the sub-stream network, the main channel reach, respectively, c^s is the specific heat capacity of the saturated zone at a constant volume, l_{il} is the latent heat of freezing.

6.4 Balance equations for unsaturated zone

Balance equation of mass for water phase:

$$\frac{d}{dt} \left(\overline{\rho_l^u} \varepsilon_l^u y^u \omega^u \right) = e_l^{uEXT} + \sum_{L=1}^{N_K} e_l^{uL} + e_l^{us} + e_l^{ub} + e_l^{uv} + e_l^{un} + e_l^{ug} + e_{li}^u , \tag{45}$$

where the l.h.s. term represents the rate of change of water storage, the terms on the r.h.s. are various water exchange terms with the external world to the watershed, neighboring REWs, saturated zone, bared zone, vegetation covered zone, snow covered zone, glacier covered zone, and ice phase respectively. Of these the first two terms can be considered as subsurface and preferred flows, and e_l^{us} equals $-e_l^{su}$, according to the jump condition (Reggiani et al., 1998, 1999), e_l^{ub} represents infiltration from the bare soil zone during a storm period when positive and capillary rise during an inter-storm period when negative, which is then evaporated into the atmosphere from the bare soil zone. Similarly, e_l^{uv} represents infiltration from the vegetated zone during the storm period when positive, and uptake by plant roots during the inter-storm period when negative, which is then transpired by vegetation, e_l^{un} and e_l^{ug} (always positive or zero) represent infiltration from snow and glacier covered zones, respectively.

Balance equation of mass for ice:

$$\frac{d}{dt}\left(\overline{\rho_i^u}\varepsilon_i^u y^u \omega^u\right) = e_{il}^u = -e_{li}^u \tag{46}$$

Balance equation of momentum for water:

$$\overline{\rho_l^u}\varepsilon_l^u y^u \omega^u \frac{d}{dt}\overline{\mathbf{v}_l^u} - \overline{\mathbf{g}_l^u \rho_l^u}\varepsilon_l^u y^u \omega^u = \mathbf{T}_l^{uEXT} + \sum_{L=1}^{N_K} \mathbf{T}_l^{uL}$$
$$, \quad + \mathbf{T}_l^{us} + \mathbf{T}_l^{ub} + \mathbf{T}_l^{uv} + \mathbf{T}_l^{un} + \mathbf{T}_l^{ug} + \mathbf{T}_{lm}^u + \mathbf{T}_{lg}^u + \mathbf{T}_{li}^u \tag{47}$$

where the terms on the l.h.s. are the inertial term and weight of water, respectively. The r.h.s. terms represent various forces: the total pressure forces acting on the mantle segments in common with the external watershed boundary and with the neighboring REWs, the forces transmitted to the saturated zone across the water table, to the bare soil zone, to the vegetated zone, the snow covered zone, and the glacier covered zone, and finally, the resultant forces exchanged with the soil matrix, gas, and the ice on the water-soil matrix, water-gas, and water-ice interfaces, respectively.

Similarly, the momentum terms of $\mathbf{T}_{lm}^u$ and $\mathbf{T}_{li}^u$ can be united into one single term $\mathbf{T}_{l(m,i)}^u$ which is denoted by $\mathbf{T}_{lm}^u$ unless otherwise confusion arises.

$$\overline{\rho_l^u}\varepsilon_l^u y^u \omega^u \frac{d}{dt}\overline{\mathbf{v}_l^u} - \overline{\mathbf{g}_l^u \rho_l^u}\varepsilon_l^u y^u \omega^u = \mathbf{T}_l^{uEXT} + \sum_{L=1}^{N_K} \mathbf{T}_l^{uL}$$
$$+ \mathbf{T}_l^{us} + \mathbf{T}_l^{ub} + \mathbf{T}_l^{uv} + \mathbf{T}_l^{un} + \mathbf{T}_l^{ug} + \mathbf{T}_{lm}^u + \mathbf{T}_{lg}^u \tag{48}$$

Similar to the saturated zone, we can write down the balance equations for heat for water, the soil matrix, ice, and gas respectively and then add them together. In the interest of brevity, only the final results for the unsaturated zone are given.

Balance equation of heat for unsaturated zone:

$$y^u \omega^u c^u \frac{d}{dt}\overline{\theta^u} - l_{il} e^u_{il} = Q^{us} + Q^{ub} + Q^{uv} + Q^{un} + Q^{ug} , \tag{49}$$

where on the l.h.s. the first term represents the rate of change of heat storage due to variation of the temperature, the second term accounts for the rate of freezing heat. The terms on the r.h.s. are REW-scale heat exchange terms with the saturated zone, bare soil zone, vegetated zone, snow covered zone, and glacier covered zone, respectively.

6.5 Balance equations for bare soil zone

The bare soil zone includes the soil matrix, liquid water, and vapor. Owing to Assumption 1, vapor disperses immediately after evaporation.

Balance equation of mass for water phase:

$$\frac{d}{dt}\left(\overline{\rho^b_l} y^b \omega^b\right) = e^{bT}_l + e^{bu}_l + e^{bt}_l + e^b_{lg} , \tag{50}$$

where the l.h.s. term represents the rate of change of depression storage, the terms on the r.h.s. account for the intensity of rainfall, water exchange rate with the unsaturated zone, with the sub-stream network, and with the vapor phase (i.e. evaporation).

Balance equation of heat for bared zone:

$$y^b \omega^b c^b \frac{d}{dt}\overline{\theta^{surf}} - l_{lg} e^b_{lg} - R_n \omega^b = Q^{bT} + Q^{bu} \tag{51}$$

where the terms on the l.h.s. are the rate of change of heat storage due to variation of temperature, the rate of latent heat transfer of vaporization, and net radiant intensity, respectively. The terms on the r.h.s. represent heat exchange rate with the atmosphere due to turbulence and the unsaturated zone, l_{lg} is the latent heat of vaporization, and R_n is the net radian intensity.

6.6 Balance equations for vegetated zone

Balance equation of mass for water phase:

$$\frac{d}{dt}\left(\overline{\rho_l^v}\varepsilon_l^v y^v \omega^v\right) = e_l^{vT} + e_l^{vu} + e_l^{vt} + e_{lg}^v , \tag{52}$$

where the l.h.s. term accounts for the rate of change of water storage (i.e. canopy interception and depression storage), the terms on the r.h.s. represent the intensity of rainfall, water exchange rate with the unsaturated zone, with the sub-stream network, and with the vapor phase (i.e. transpiration).

Balance equation of heat for vegetation covered zone:

$$y^v \omega^v c^v \frac{d}{dt}\overline{\theta^{surf}} - l_{lg} e_{lg}^v - R_n \omega^v = Q^{vT} + Q^{vu} , \tag{53}$$

where the terms on the l.h.s. are the rate of change of heat storage due to temperature variation, the rate of latent heat transfer of vaporization, and net radian intensity, respectively. The terms on the r.h.s. represent heat exchange with the atmosphere due to turbulence and the unsaturated zone, l_{lg} is the latent heat of vaporization, and R_n is the intensity of radiation.

6.7 Balance equations for snow covered zone

Balance equation of mass for water phase:

$$\frac{d}{dt}\left(\overline{\rho_l^n}\varepsilon_l^n y^n \omega^n\right) = e_l^{nT} + e_l^{nu} + e_l^{nt} + e_{lg}^n + e_{ln}^n , \tag{54}$$

where the l.h.s. term accounts for the rate of change of water storage, the terms on the r.h.s. represent the intensity of rainfall, water exchange rate with the unsaturated zone, with the sub-stream network, with the vapor phase (i.e. evaporation), and with the snow phase (i.e. melting).

Balance equation of mass for snow phase:

$$\frac{d}{dt}\left(\overline{\rho_n^n}\varepsilon_n^n y^n \omega^n\right) = e_n^{nT} + e_{ng}^n + e_{nl}^n \,, \tag{55}$$

where the l.h.s. term is the rate of change of snow storage, the terms on the r.h.s. represent the intensity of snowfall, snow exchange rate with the vapor phase (i.e. sublimation) and with the water phase (i.e. melting). According to the jump condition, $e_{nl}^n = -e_{ln}^n$.

Balance equation of heat for snow covered zone:

$$y^n \omega^n c^n \frac{d}{dt}\overline{\theta^n} - l_{lg} e_{lg}^n - l_{ng} e_{ng}^n - l_{nl} e_{nl}^n - R_n \omega^n = Q^{nT} + Q^{nu} \,, \tag{56}$$

where the terms on the l.h.s. are the rate of change of heat storage due to temperature variation, the rate of latent heat transfer of vaporization, the rate of latent heat transfer of sublimation, the rate of heat transfer of melting, and net radiant intensity, respectively. The terms on the r.h.s. represent heat exchange rate with the atmosphere due to turbulence and the unsaturated zone, l_{lg} is the latent heat of vaporization, l_{ng} is the latent heat of sublimation, l_{nl} is the latent heat of melting, and R_n is the intensity of radiation.

6.8 Balance equations for glacier covered zone

Balance equation of mass for water phase:

$$e_l^{gT} + e_l^{gu} + e_l^{gt} + e_{lg}^g + e_{li}^g = 0 \tag{57}$$

where the terms on the l.h.s. account for the intensity of rainfall, water exchange rate with unsaturated zone, with the sub-stream network, with the vapor phase (i.e.

evaporation), and with the ice phase (i.e. melting or freezing). Here we omit the water storage capacity of the glacier covered zone.

Balance equation of mass for ice phase:

$$\frac{d}{dt}\left(\overline{\rho_i^g} y^g \omega^g\right) = e_{ig}^g + e_{il}^g , \tag{58}$$

where the terms on the r.h.s. represent the rates of sublimation and freezing respectively.

Balance equation of heat for glacier covered zone:

$$y^g \omega^g c^g \frac{d}{dt}\overline{\theta^g} - l_{lg} e_{lg}^g - l_{ig} e_{ig}^g - l_{il} e_{il}^g - R_n \omega^g = Q^{gT} + Q^{gu} , \tag{59}$$

where the terms on the l.h.s. are the rate of change of heat storage due to variation of temperature, the rate of latent heat transfer of vaporization, the rate of latent heat transfer of sublimation, the rate of latent heat transfer of melting, and net radian intensity, respectively. The terms on the r.h.s. represent heat exchange rate with the atmosphere due to turbulence and the unsaturated zone, l_{lg} is the latent heat of vaporization, l_{ig} is the latent heat of sublimation, l_{il} is the latent heat of melting, and R_n is the intensity of radiation.

6.9 Balance equations for main channel reach

Balance equation of mass for water phase:

$$\frac{d}{dt}\left(\overline{\rho}_l^r m^r \xi^r\right) = e_l^{rT} + e_l^{rEXT} + \sum_{L=1}^{N_K} e_l^{rL} + e_l^{rt} + e_l^{rs} + e_{lg}^r \tag{60}$$

where the l.h.s. term represents the rate of change of water storage, the terms on the r.h.s. are the intensity of rainfall, various water exchange rate terms with the external world to the watershed, with neighboring REWs, with the sub-stream network, with the saturated zone, and with the vapor phase (i.e. evaporation), respectively.

Balance equation of momentum for water phase:

$$\left(\overline{\rho_l^r} m^r \xi^r\right) \frac{d}{dt} \overline{\mathbf{v}_l^r} - \mathbf{g}_l^r \overline{\rho_l^r} m^r \xi^r = \mathbf{T}_l^{rEXT} + \sum_{L=1}^{N_K} \mathbf{T}_l^{rL} + \mathbf{T}_l^{rT} + \mathbf{T}_l^{rt} + \mathbf{T}_l^{rs}, \tag{61}$$

where the terms on the l.h.s. are the inertial term and weight of water, respectively. The r.h.s. terms represents various forces: the total pressure forces acting on the channel cross sections in common with the external watershed boundary and with the neighboring REWs, the forces transmitted to the atmosphere, to the sub-stream network, and to the saturated zone, respectively.

Balance equation of heat for main channel reach:

$$\overline{\rho_l^r} m^r \xi^r \frac{d}{dt} \overline{\theta^r} - l_{lg} e_{lg}^r - R_n \omega^r = Q^{rT} + Q^{rs} \tag{62}$$

where the terms on the l.h.s. are the rate of change of heat storage due to variation of temperature, the rate of latent heat transfer of vaporization, and net radian intensity, respectively. The terms on the r.h.s. represent heat exchange rate with the atmosphere due to turbulence and the saturated zone, l_{lg} is the latent heat of vaporization, and R_n is the intensity of radiation.

6.10 Balance equations for sub stream network

Balance equation of mass for water phase:

$$\frac{d}{dt}\left(\overline{\rho_l^t} y^t \omega^t\right) = e_l^{tT} + e_l^{tb} + e_l^{tv} + e_l^{tn} + e_l^{tg} + e_l^{ts} + e_l^{tr} + e_{lg}^t, \tag{63}$$

where the l.h.s. term represents the rate of change of water storage, the terms on the r.h.s. are the intensity of rainfall, various water exchange rate terms with the bare soil zone, with the vegetated zone, with the snow covered zone, with the glacier covered zone, with the saturated zone, with the main channel reach, and with the vapor phase (i.e. evaporation), respectively.

Balance equation of momentum for water phase:

$$\left(\overline{\rho_l^t} y^t \omega^t\right) \frac{d}{dt} \overline{\boldsymbol{v}_l^t} - \overline{\boldsymbol{g}_l^t \rho_l^t} y^t \omega^t = \boldsymbol{T}_l^{tT} + \boldsymbol{T}_l^{tb} + \boldsymbol{T}_l^{tv} + \boldsymbol{T}_l^{tn} + \boldsymbol{T}_l^{tg} + \boldsymbol{T}_l^{ts} + \boldsymbol{T}_l^{tr}, \tag{64}$$

where the terms on the l.h.s. are the inertial term and weight of water, respectively. The r.h.s. terms represent various forces: the forces transmitted to the atmosphere, to the bare soil zone, to the vegetated zone, to the snow covered zone, to the glacier covered zone, to the saturated zone, and to the main channel reach, respectively.

Balance equation of heat for sub stream network:

$$y^t \omega^t c^t \frac{d}{dt} \overline{\theta^r} - l_{lg} e_{lg}^t - R_n \omega^t = Q^{tT} + Q^{ts}, \tag{65}$$

where the terms on the l.h.s. are the rate of change of heat storage due to variation of temperature, the rate of latent heat transfer of vaporization, and net radian intensity, respectively. The terms on the r.h.s. represent heat exchange rate with the atmosphere due to turbulence and the saturated zone, l_{lg} is the latent heat of vaporization, and R_n is the intensity of radiation.

7 Conclusions

The REW theory is a novel watershed hydrological modeling approach whose equations are applicable directly to the spatial scale of the watershed. The pioneering work

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by Reggiani et al. (1998, 1999) provides the unifying framework for the REW approach and the definition of REW is fundamental to it. As an initial attempt, Reggiani et al.'s definition precludes hydrological processes driven by or intimately related to energy balances, such as evapotranspiration, freezing, and thawing, from being modeled in a physically reasonable way. After a revision of Reggiani et al.'s definition of REW, this paper derives the fundamental equations all over again, by paying particular attention to energy balance processes, in order to extend the applicability of the REW approach.

In our new definition, a REW is separated into surface and subsurface layers which are further divided into six sub-regions and two sub-regions, respectively. Soil ice, vapor, vegetation, snow, and glacier ice are added to the existing system, including water, gas, and the soil matrix. Owing to the vapor phase, evaporation and transpiration can be modeled separately in a physical manner. The original separation of saturated overland flow and concentrated overland flow zones is abandoned. As a result, it is no longer necessary to divide surface runoff into two different components. Surface runoff is generated on the six surface sub-regions and its magnitude is equals to the rainfall minus infiltration capacity (which depends on soil type and soil moisture and is represented by constitutive relationships). Subsurface flow and preferred flow are embedded in the mass exchange term between the unsaturated zone and the neighboring REWs or the external world. Groundwater flow is represented by the exchange term between saturated zone and the neighboring REWs or the external world. Total surface runoff can be divided the into infiltration excess and saturation excess ones according to the status of soil saturation, where needed.

The general form of time-averaged conservation laws of mass, momentum, energy, and entropy at the spatial scale of REW is then formulated. After a series of assumptions, the general form is applied to derive the balance equations for each phase in each sub-region. There are in total 24 balance equations, four of which are vector momentum balance equations. For a watershed with M discrete REWs, we get finally a system of M×24 coupled equations.

Our procedure is more concise and is more easily applied when it is desired to

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include new sub-regions and phases into the approach. If we want to incorporate into the model sub-regions representing the effect of human activities on hydrological processes, such as the presence of lakes and reservoirs, for example, what we should do is simply separate the reservoir from the sub-stream network zone and add it to the surface layer. Then we can apply the general form of averaged balance equations presented in Sect. 5.2 to all phases contained within the reservoir sub-region. New equations are then coupled into the equation set.

The system of equations has a redundant number of variables for which constitutive relationships are necessary. It is the unalterable principle in continuum mechanics where constitutive relationships account for the characteristics of the materials. Currently, Reggiani et al. (2005) propose a set of closure relationships based on the exploitation of the second law, and Lee et al. (2005a, b) propose their closure relationships based on various upscaling methods. The additional relationships required to close these new set of balance equations will be pursued in a subsequent paper.

Appendix

A. Time averaged general form of conservation laws for mass, momentum, energy and entropy

In Sect. 5.2, we obtained the general form of conservation laws, i.e., Eq. (29), based on microscopic quantities. After averaging Eq. (29) in time by integrating each term separately over the interval $(t-\Delta t, t+\Delta t)$ and dividing by $2\Delta t$ we get

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$$
\overbrace{\frac{1}{2\Delta t}\int_{t-\Delta t}^{t+\Delta t}\left(\frac{\partial}{\partial t}\int_{V_\alpha^j}\rho_\alpha^j\psi_\alpha^j dV\right)d\tau}^{\text{temporal derivation of } \phi}
$$

$$
+\overbrace{\sum_{P=EXT,L,T,B,i}^{L=1\ldots N_K,i\neq j}\frac{1}{2\Delta t}\int_{t-\Delta t}^{t+\Delta t}\int_{S^{jP}}\rho_\alpha^j\psi_\alpha^j\left(\boldsymbol{v}_\alpha^j-\boldsymbol{w}_\alpha^{jP}\right)\cdot\gamma_a^j d\boldsymbol{A}d\tau+\sum_{\beta\neq\alpha}\frac{1}{2\Delta t}\int_{t-\Delta t}^{t+\Delta t}\int_{S_{\alpha\beta}^j}\rho_\alpha^j\psi_\alpha^j\left(\boldsymbol{v}_\alpha^j-\boldsymbol{w}_{\alpha\beta}^j\right)\cdot d\boldsymbol{A}d\tau}^{\text{spatial derivation of } \phi}
$$

$$
-\overbrace{\sum_{P=EXT,L,T,B,i}^{L=1\ldots N_K,i\neq j}\frac{1}{2\Delta t}\int_{t-\Delta t}^{t+\Delta t}\int_{S^{jp}}\boldsymbol{i}\cdot\gamma_a^j d\boldsymbol{A}d\tau-\sum_{\beta\neq\alpha}\frac{1}{2\Delta t}\int_{t-\Delta t}^{t+\Delta t}\int_{S_{\alpha\beta}^j}\boldsymbol{i}\cdot d\boldsymbol{A}d\tau}^{\text{influx}}
$$

$$
-\overbrace{\frac{1}{2\Delta t}\int_{t-\Delta t}^{t+\Delta t}\int_{V_\alpha^j}\left(\rho_\alpha^j f+G\right)dVd\tau}^{\text{source or sink term}}=0 \qquad (66)
$$

In the following, after presenting the definition of fluctuations and associated lemmas, we derive the time averaged form of each term in the Eq. (66) in turn.

(1) Definition and lemmas about fluctuations of conserved quantity ϕ

From the microscopic point of view, the kinetic quantities of all phases within each sub-region fluctuate around the average value which behaves similarly with turbulent flow. It is impossible and unnecessary to obtain their instantaneous value on the microscopic scale. The temporal and spatial averaging quantities are more important for watershed hydrological modeling. For this purpose, the actual movement is decomposed into two components, one is the time averaged quantity, and the other is the fluctuating quantity or residual. This can be expressed in an equation as follows:

$$\psi_\alpha^j = \overline{\psi_\alpha^j} + \widetilde{\psi_\alpha^j}, \tag{67}$$

where ψ_α^j is the instantaneous value of the physical quantity $\boldsymbol{\phi}$, $\widetilde{\psi_\alpha^j}$ is the fluctuating value or residual, and $\overline{\psi_\alpha^j}$ is the time-averaged value, which is defined in Eq. (18) and Eq. (22). For convenience, we give the definitions again.

$$\overline{\psi_\alpha^j} = \frac{1}{2\Delta t \overline{\rho_\alpha^j} \varepsilon_\alpha^j y^j \omega^j \sum} \int_{t-\Delta t}^{t+\Delta t} \int_{V^j} \rho_\alpha^j \psi_\alpha^j \gamma_a^j dV d\tau, j \neq r$$
$$\overline{\psi_\alpha^r} = \frac{1}{2\Delta t \overline{\rho_\alpha^r} m^r \xi^r \sum} \int_{t-\Delta t}^{t+\Delta t} \int_{V^r} \rho_\alpha^r \psi_a^r \gamma_a^r dV d\tau. \tag{68}$$

According to Eq. (68), the time-averaged value of $\widetilde{\psi_\alpha^j}$ must be zero,

$$\widetilde{\psi_\alpha^j} = \frac{1}{2\Delta t \varepsilon_\alpha^j y^j \rho_\alpha^j \omega^j \sum} \int_{t-\Delta t}^{t+\Delta t} \int_{V^j} \rho_\alpha^j \widetilde{\psi_\alpha^j} \gamma_a^j dV d\tau = 0. \tag{69}$$

About the fluctuation of physical quantity $\boldsymbol{\phi}$, we give the following lemmas for later use (for the formulation of the time averaged energy conservation equations).

Lemma 1 The time averaged value of the product of two instantaneous values can be calculated by the formula

$$\overline{f_1 f_2} = \overline{f_1}\,\overline{f_2} + \overline{\widetilde{f_1}\widetilde{f_2}} \tag{70}$$

Proof:

$$\overline{f_1 f_2}$$
$$= \overline{\left(\overline{f_1} + \tilde{f}_1\right)\left(\overline{f_2} + \tilde{f}_2\right)}$$
$$= \overline{\left(\overline{f_1}\,\overline{f_2} + \overline{f_1}\tilde{f}_2 + \overline{f_2}\tilde{f}_1 + \tilde{f}_1\tilde{f}_2\right)}$$
$$= \overline{\overline{f_1}\,\overline{f_2}} + \overline{\overline{f_1}\tilde{f}_2} + \overline{\overline{f_2}\tilde{f}_1} + \overline{\tilde{f}_1\tilde{f}_2}$$
$$= \overline{f_1}\,\overline{f_2} + \overline{f_1}\,\overline{\tilde{f}_2} + \overline{f_2}\,\overline{\tilde{f}_1} + \overline{\tilde{f}_1\tilde{f}_2}$$
$$= \overline{f_1}\,\overline{f_2} + \overline{\tilde{f}_1\tilde{f}_2}$$

Lemma 2 The fluctuation value of the product of two instantaneous values can be calculated by the formula

$$\widetilde{f_1 f_2} = \overline{f_1}\tilde{f}_2 + \tilde{f}_1\overline{f_2} + \widetilde{\tilde{f}_1\tilde{f}_2} \tag{71}$$

Proof:

$$\widetilde{\overline{f_1}\tilde{f}_2} = \overline{f_1}\tilde{f}_2 - \overline{\overline{f_1}\tilde{f}_2} = \overline{f_1}\tilde{f}_2 - \overline{f_1}\,\overline{\tilde{f}_2} = \overline{f_1}\tilde{f}_2 \tag{72}$$

$$\widetilde{f_1 f_2}$$
$$= \widetilde{\left(\overline{f_1} + \tilde{f}_1\right)\left(\overline{f_2} + \tilde{f}_2\right)}$$
$$= \widetilde{\left(\overline{f_1}\,\overline{f_2} + \overline{f_1}\tilde{f}_2 + \tilde{f}_1\overline{f_2} + \tilde{f}_1\tilde{f}_2\right)}$$
$$= \widetilde{\overline{f_1}\,\overline{f_2}} + \widetilde{\overline{f_1}\tilde{f}_2} + \widetilde{\tilde{f}_1\overline{f_2}} + \widetilde{\tilde{f}_1\tilde{f}_2}$$
$$= \overline{f_1}\tilde{f}_2 + \tilde{f}_1\overline{f_2} + \widetilde{\tilde{f}_1\tilde{f}_2}$$

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(2) Temporal derivation term of the physical quantity $\boldsymbol{\phi}$

The first term on the l.h.s. of Eq. (66) is the temporal derivative of the physical quantity $\boldsymbol{\phi}$. According to the well-known theorem (see Whitaker, 1981, pp. 192–193), the order of time integration and time differentiation may be changed and the results integrated as follows:

$$\frac{1}{2\Delta t}\int_{t-\Delta t}^{t+\Delta t}\left(\frac{\partial}{\partial t}\int_{V_\alpha^j}\rho_\alpha^j\psi_\alpha^j dV\right)d\tau=\frac{1}{2\Delta t}\frac{\partial}{\partial t}\int_{t-\Delta t}^{t+\Delta t}\int_{V_\alpha^j}\rho_\alpha^j\psi_\alpha^j dV d\tau$$
$$=\frac{\partial}{\partial t}\left(\frac{1}{2\Delta t}\int_{t-\Delta t}^{t+\Delta t}\int_{V^j}\rho_\alpha^j\psi_\alpha^j\gamma_a^j dV d\tau\right)=\frac{\partial}{\partial t}\left(\overline{\psi_\alpha^j\rho_\alpha^j}\varepsilon_\alpha^j y^j\omega^j\Sigma\right) \tag{73}$$

(3) Spatial derivation term of the physical quantity $\boldsymbol{\phi}$

The second and third terms on the l.h.s. of Eq. (66) are the spatial derivative terms of physical quantity $\boldsymbol{\phi}$, i.e. exchange rate of the physical quantity $\boldsymbol{\phi}$ through the interface S_α^{jP} ($P{=}EXT,L,T,B,i,L{=}1...N_K,i{\neq}j$) and $S_{\alpha\beta}^j$ ($\beta{\neq}\alpha$), respectively. According to Eq. (67) to Eq. (70) and the definitions of REW-scale mass exchange terms through interfaces (see Eq. (26) and Eq. (27)), the exchange rate of $\boldsymbol{\phi}$ through S_α^{jP} (the second term on the l.h.s. of Eq. (66)) can be formulated as follows:

$$\frac{1}{2\Delta t}\int_{t-\Delta t}^{t+\Delta t}\int_{S^{jP}}\rho_\alpha^j\psi_\alpha^j\left(\mathbf{v}_\alpha^j-\mathbf{w}_\alpha^{jP}\right)\cdot\gamma_a^j d\mathbf{A}d\tau$$
$$=\frac{1}{2\Delta t}\int_{t-\Delta t}^{t+\Delta t}\int_{S^{jP}}\rho_\alpha^j\left(\overline{\psi_\alpha^j}+\widetilde{\psi_\alpha^j}\right)\left(\mathbf{v}_\alpha^j-\mathbf{w}_\alpha^{jP}\right)\cdot\gamma_a^j d\mathbf{A}d\tau$$
$$=\frac{1}{2\Delta t}\int_{t-\Delta t}^{t+\Delta t}\int_{S^{jP}}\rho_\alpha^j\overline{\psi_\alpha^j}\left(\mathbf{v}_\alpha^j-\mathbf{w}_\alpha^{jP}\right)\cdot\gamma_a^j d\mathbf{A}d\tau+\frac{1}{2\Delta t}\int_{t-\Delta t}^{t+\Delta t}\int_{S^{jP}}\rho_\alpha^j\widetilde{\psi_\alpha^j}\left(\mathbf{v}_\alpha^j-\mathbf{w}_\alpha^{jP}\right)\cdot\gamma_a^j d\mathbf{A}d\tau$$

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$$= \overline{\psi^j_\alpha} \overbrace{\frac{1}{2\Delta t}\int_{t-\Delta t}^{t+\Delta t}\int_{S^{jP}} \rho^j_\alpha \left(\boldsymbol{v}^j_\alpha - \boldsymbol{w}^{jP}_\alpha\right)\cdot \gamma^j_a d\boldsymbol{A} d\tau}^{\text{according to Eq. (26)}} + \frac{1}{2\Delta t}\int_{t-\Delta t}^{t+\Delta t}\int_{S^{jP}} \rho^j_\alpha \widetilde{\psi^j_\alpha} \left(\boldsymbol{v}^j_\alpha - \boldsymbol{w}^{jP}_\alpha\right)\cdot \gamma^j_a d\boldsymbol{A} d\tau$$

$$= -\overline{\psi^j_\alpha} e^{jP}_\alpha \Sigma + \frac{1}{2\Delta t}\int_{t-\Delta t}^{t+\Delta t}\int_{S^{jP}} \rho^j_\alpha \widetilde{\psi^j_\alpha} \left(\boldsymbol{v}^j_\alpha - \boldsymbol{w}^{jP}_\alpha\right)\cdot \gamma^j_a d\boldsymbol{A} d\tau \tag{74}$$

Similarly, the exchange rate of $\boldsymbol{\phi}$ through $S^j_{\alpha\beta}$ (the third term on the l.h.s. of Eq. 66) can be formulated as:

$$\frac{1}{2\Delta t}\int_{t-\Delta t}^{t+\Delta t}\int_{S^j_{\alpha\beta}} \rho^j_\alpha \psi^j_\alpha \left(\boldsymbol{v}^j_\alpha - \boldsymbol{w}^j_{\alpha\beta}\right)\cdot \gamma^j_a d\boldsymbol{A} d\tau$$

$$= -\overline{\psi^j_\alpha} e^j_{\alpha\beta} \Sigma + \frac{1}{2\Delta t}\int_{t-\Delta t}^{t+\Delta t}\int_{S^j_{\alpha\beta}} \rho^j_\alpha \widetilde{\psi^j_\alpha} \left(\boldsymbol{v}^j_\alpha - \boldsymbol{w}^j_{\alpha\beta}\right)\cdot \gamma^j_a d\boldsymbol{A} d\tau \tag{75}$$

(4) Convective and non-convective terms of the physical quantity $\boldsymbol{\phi}$

Substitution Eq. (73), Eq. (74), and Eq. (75) into Eq. (66) yields:

$$\frac{\partial}{\partial t}\left(\overline{\psi^j_\alpha \rho^j_\alpha} \varepsilon^j_\alpha y^j \omega^j \Sigma\right) + \sum_{P=EXT,L,T,B,i}^{L=1\ldots N_K, i\neq j} \left(-\overline{\psi^j_\alpha} e^{jP}_\alpha \Sigma + \frac{1}{2\Delta t}\int_{t-\Delta t}^{t+\Delta t}\int_{S^{jP}} \rho^j_\alpha \widetilde{\psi^j_\alpha} \left(\boldsymbol{v}^j_\alpha - \boldsymbol{w}^{jP}_\alpha\right)\cdot \gamma^j_a d\boldsymbol{A} d\tau\right)$$

$$+ \sum_{\beta\neq\alpha}\left(-\overline{\psi^j_\alpha} e^j_{\alpha\beta}\Sigma + \frac{1}{2\Delta t}\int_{t-\Delta t}^{t+\Delta t}\int_{S^j_{\alpha\beta}} \rho^j_\alpha \widetilde{\psi^j_\alpha}\left(\boldsymbol{v}^j_\alpha - \boldsymbol{w}^j_{\alpha\beta}\right)\cdot d\boldsymbol{A} d\tau\right)$$

$$- \sum_{P=EXT,L,T,B,i}^{L=1\ldots N_K, i\neq j} \frac{1}{2\Delta t}\int_{t-\Delta t}^{t+\Delta t}\int_{S^{jP}} \boldsymbol{i}\cdot \gamma^j_a d\boldsymbol{A} d\tau$$

$$-\sum_{\beta\neq\alpha}\frac{1}{2\Delta t}\int_{t-\Delta t}^{t+\Delta t}\int_{S_{\alpha\beta}^j}\boldsymbol{i}\cdot d\boldsymbol{A}d\tau-\frac{1}{2\Delta t}\int_{t-\Delta t}^{t+\Delta t}\int_{V_\alpha^j}\left(\rho_\alpha^j f+G\right)dVd\tau=0\Rightarrow$$

$$\frac{\partial}{\partial t}\left(\overline{\psi_\alpha^j\rho_\alpha^j\varepsilon_\alpha^j y^j\omega^j}\Sigma\right)-\sum_{P=EXT,L,T,B,i}^{L=1\ldots N_K,i\neq j}\overline{\psi_\alpha^j}e_\alpha^{jP}\Sigma-\sum_{\beta\neq\alpha}\overline{\psi_\alpha^j}e_{\alpha\beta}^j\Sigma$$

$$+\sum_{P=EXT,L,T,B,i}^{L=1\ldots N_K,i\neq j}\frac{1}{2\Delta t}\int_{t-\Delta t}^{t+\Delta t}\int_{S^{jP}}\rho_\alpha^j\widetilde{\psi_\alpha^j}\left(\boldsymbol{v}_\alpha^j-\boldsymbol{w}_\alpha^{jP}\right)\cdot\gamma_a^j d\boldsymbol{A}d\tau-\sum_{P=EXT,L,T,B,i}^{L=1\ldots N_K,i\neq j}\frac{1}{2\Delta t}\int_{t-\Delta t}^{t+\Delta t}\int_{S^{jP}}\boldsymbol{i}\cdot\gamma_a^j d\boldsymbol{A}d\tau$$

$$+\sum_{\beta\neq\alpha}\frac{1}{2\Delta t}\int_{t-\Delta t}^{t+\Delta t}\int_{S_{\alpha\beta}^j}\rho_\alpha^j\widetilde{\psi_\alpha^j}\left(\boldsymbol{v}_\alpha^j-\boldsymbol{w}_{\alpha\beta}^j\right)\cdot d\boldsymbol{A}d\tau-\sum_{\beta\neq\alpha}\frac{1}{2\Delta t}\int_{t-\Delta t}^{t+\Delta t}\int_{S_{\alpha\beta}^j}\boldsymbol{i}\cdot d\boldsymbol{A}d\tau$$

$$-\frac{1}{2\Delta t}\int_{t-\Delta t}^{t+\Delta t}\int_{V_\alpha^j}\left(\rho_\alpha^j f+G\right)dVd\tau=0\Rightarrow$$

$$\frac{\partial}{\partial t}\left(\overline{\psi_\alpha^j\rho_\alpha^j\varepsilon_\alpha^j y^j\omega^j}\sum\right)-\overbrace{\left(\sum_{P=EXT,L,T,B,i}^{L=1\ldots N_K,i\neq j}\overline{\psi_\alpha^j}e_\alpha^{jP}\Sigma+\sum_{\beta\neq\alpha}\overline{\psi_\alpha^j}e_{\alpha\beta}^j\Sigma\right)}^{\text{convective term}}+$$

$$\overbrace{\sum_{P=EXT,L,T,B,i}^{L=1\ldots N_K,i\neq j}\frac{1}{2\Delta t}\int_{t-\Delta t}^{t+\Delta t}\int_{S^{jP}}\left[\rho_\alpha^j\widetilde{\psi_\alpha^j}\left(\boldsymbol{v}_\alpha^j-\boldsymbol{w}_\alpha^{jP}\right)-\boldsymbol{i}\right]\cdot\gamma_a^j d\boldsymbol{A}d\tau}^{\text{non-convective term through }S^{jP}}+$$

$$\overbrace{\sum_{\beta\neq\alpha}\frac{1}{2\Delta t}\int_{t-\Delta t}^{t+\Delta t}\int_{S^j_{\alpha\beta}}\left[\rho^j_\alpha\widetilde{\psi^j_\alpha}\left(\boldsymbol{v}^j_\alpha-\boldsymbol{w}^j_{\alpha\beta}\right)-\boldsymbol{i}\right]\cdot d\boldsymbol{A}d\tau}^{\text{non-convective term through } S^j_{\alpha\beta}}-$$

$$\overbrace{\frac{1}{2\Delta t}\int_{t-\Delta t}^{t+\Delta t}\int_{V^j_\alpha}\left(\rho^j_\alpha f+G\right)dVd\tau}^{\text{source or sink term}}=0 \tag{76}$$

In the interest of brevity, we make the following definitions:

Definition 13: The non-convective term of physical quantity $\boldsymbol{\phi}$ through interface S^{jP}_α

$$I^{jP}_\alpha=\frac{1}{2\Delta t\Sigma}\int_{t-\Delta t}^{t+\Delta t}\int_{S^{jP}}\left[\boldsymbol{i}-\rho^j_\alpha\widetilde{\psi^j_\alpha}\left(\boldsymbol{v}^j_\alpha-\boldsymbol{w}^{jP}_\alpha\right)\right]\cdot\gamma^j_a d\boldsymbol{A}d\tau$$
$$P=EXT,L,T,B,i,\ \mathrm{L}=1...N_K,i\neq j \tag{77}$$

Definition 14: The non-convective term of physical quantity $\boldsymbol{\phi}$ through interface $S^j_{\alpha,\beta}$

$$I^j_{\alpha\beta}=\frac{1}{2\Delta t\Sigma}\int_{t-\Delta t}^{t+\Delta t}\int_{S^j_{\alpha\beta}}\left[\boldsymbol{i}-\rho^j_\alpha\widetilde{\psi^j_\alpha}\left(\boldsymbol{v}^j_\alpha-\boldsymbol{w}^j_{\alpha\beta}\right)\right]\cdot d\boldsymbol{A}d\tau,\ \beta\neq a \tag{78}$$

Definition 15: The time-averaged generation rate of α phase in $B^j(k)$ per unit mass as:

$$\overline{f^j_\alpha}=\frac{1}{2\Delta t\overline{\rho^j_\alpha}\varepsilon^j_\alpha y^j\omega^j\sum}\int_{t-\Delta t}^{t+\Delta t}\int_{V^j}\rho^j_\alpha f^j_\alpha\gamma^j_a dVd\tau,j\neq r \tag{79}$$

Definition 16: The time-averaged generation rate of α phase in $B^r(k)$ per unit mass as:

$$\overline{f^r_\alpha}=\frac{1}{2\Delta t\overline{\rho^r_\alpha}m^r\xi^r\sum}\int_{t-\Delta t}^{t+\Delta t}\int_{V^r}\rho^r_\alpha f^r_a\gamma^r_a dVd\tau \tag{80}$$

Definition 17: The time-averaged generation rate of α phase in $B^j(k)$ per unit volume as:

$$\overline{G_\alpha^j} = \frac{1}{2\Delta t \varepsilon_\alpha^j y^j \omega^j \sum} \int_{t-\Delta t}^{t+\Delta t} \int_{V^j} G_\alpha^j \gamma_a^j dV d\tau, j \neq r \tag{81}$$

Definition 18: The time-averaged generation rate of α phase in $B^r(k)$ per unit volume as:

$$\overline{G_\alpha^r} = \frac{1}{2\Delta t m^r \xi^r \sum} \int_{t-\Delta t}^{t+\Delta t} \int_{V^r} G_a^r \gamma_a^r dV d\tau \tag{82}$$

Substitution Eq. (77) to Eq. (82) into Eq. (76) which is then divided by Σ yields

$$\overbrace{\frac{\partial}{\partial t}\left(\overline{\psi_\alpha^j \rho_\alpha^j} \varepsilon_\alpha^j y^j \omega^j\right)}^{\text{temporal derivation term}} - \overbrace{\left(\overline{f_\alpha^j \rho_\alpha^j} \varepsilon_\alpha^j y^j \omega^j + \overline{G_\alpha^j} \varepsilon_\alpha^j y^j \omega^j\right)}^{\text{source or sink term}}$$

$$- \overbrace{\left(\sum_{P=EXT,L,T,B,i}^{L=1\ldots N_K, i \neq j} \overline{\psi_\alpha^j} e_\alpha^{jP} + \sum_{\beta \neq \alpha} \overline{\psi_\alpha^j} e_{\alpha\beta}^j\right)}^{\text{convective term}} - \overbrace{\left(\sum_{P=EXT,L,T,B,i}^{L=1\ldots N_K, i \neq j} I_\alpha^{jP} + \sum_{\beta \neq \alpha} I_{\alpha\beta}^j\right)}^{\text{non-convective term}} = 0 \tag{83}$$

(5) General form of time averaged conservation equations

General form of mass conservation equation

The general form of mass conservation equation for α phase within j sub-region can be derived according to Table 5 such that $\psi=1$, $i=0$, $f=0$ and $G=0$ from Eq. (83).

$$\frac{\partial}{\partial t}\left(\overline{\rho_\alpha^j} \varepsilon_\alpha^j y^j \omega^j\right) = \sum_{p=ext,l,T,B,i}^{l=1\ldots N_k, i \neq j} e_\alpha^{jp} + \sum_{\beta \neq \alpha} e_{\alpha\beta}^j \tag{84}$$

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General form of momentum conservation equation

According to the chain rule, the first term on the l.h.s. of Eq. (83) can be decomposed as $\overline{\psi_\alpha^j}\frac{\partial}{\partial t}\left(\overline{\rho_\alpha^j}\varepsilon_\alpha^j y^j\omega^j\right)+\left(\overline{\rho_\alpha^j}\varepsilon_\alpha^j y^j\omega^j\right)\frac{\partial}{\partial t}\left(\overline{\psi_\alpha^j}\right)$, then Eq. (83) can be rewritten as

$$\overline{\psi_\alpha^j}\frac{\partial}{\partial t}\left(\overline{\rho_\alpha^j}\varepsilon_\alpha^j y^j\omega^j\right)+\left(\overline{\rho_\alpha^j}\varepsilon_\alpha^j y^j\omega^j\right)\frac{\partial}{\partial t}\left(\overline{\psi_\alpha^j}\right)$$
$$=\overline{f_\alpha^j\rho_\alpha^j}\varepsilon_\alpha^j y^j\omega^j+\overline{G_\alpha^j}\varepsilon_\alpha^j y^j\omega^j+\sum_{P=EXT,L,T,B,i}^{L=1\ldots N_K,i\neq j}\overline{\psi_\alpha^j}e_\alpha^{jP}+\sum_{\beta\neq\alpha}\overline{\psi_\alpha^j}e_{\alpha\beta}^j+\sum_{P=EXT,L,T,B,i}^{L=1\ldots N_K,i\neq j}I_\alpha^{jP}+\sum_{\beta\neq\alpha}I_{\alpha\beta}^j \quad (85)$$

Multiplication of the mass conservation Eq. (84) by the $\overline{\psi_\alpha^j}$ and subsequent subtraction from Eq. (85) gives the general form of time averaged conservation equations of momentum, energy, and entropy as follows:

$$\left(\overline{\rho_\alpha^j}\varepsilon_\alpha^j y^j\omega^j\right)\frac{\partial}{\partial t}\left(\overline{\psi_\alpha^j}\right)=\overline{f_\alpha^j\rho_\alpha^j}\varepsilon_\alpha^j y^j\omega^j+\overline{G_\alpha^j}\varepsilon_\alpha^j y^j\omega^j+\sum_{P=EXT,L,T,B,i}^{L=1\ldots N_K,i\neq j}I_\alpha^{jP}+\sum_{\beta\neq\alpha}I_{\alpha\beta}^j \quad (86)$$

Therefore, the general form of momentum conservation equation for α phase within j sub-region can be derived according to Table 5 such that $\psi=\boldsymbol{v}$, $i=\boldsymbol{t}$, $f=\boldsymbol{g}$ and $G=0$ from Eq. (86) (for clarity, non-convective momentum is denoted by the symbol $\boldsymbol{T}$):

$$\left(\overline{\rho_\alpha^j}\varepsilon_\alpha^j y^j\omega^j\right)\frac{d}{dt}\left(\overline{\boldsymbol{v}_\alpha^j}\right)=\overline{\boldsymbol{g}_\alpha^j\rho_\alpha^j}\varepsilon_\alpha^j y^j\omega^j+\sum_{P=EXT,L,T,B,i}^{L=1\ldots N_K,i\neq j}\boldsymbol{T}_\alpha^{jP}+\sum_{\beta\neq\alpha}\boldsymbol{T}_{\alpha\beta}^j \quad (87)$$

where:

$$\boldsymbol{T}_\alpha^{jP}=\frac{1}{2\Delta t\Sigma}\int_{t-\Delta t}^{t+\Delta t}\int_{S^{jP}}\left[\boldsymbol{t}-\rho_\alpha^j\widetilde{\boldsymbol{v}_\alpha^j}\left(\boldsymbol{v}_\alpha^j-\boldsymbol{w}_\alpha^{jP}\right)\right]\cdot\gamma_a^j d\boldsymbol{A}d\tau,$$
$$P=EXT,L,T,B,i,L=1\ldots N_k,i\neq j \quad (88)$$

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$$\boldsymbol{T}^j_{\alpha\beta} = \frac{1}{2\Delta t \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_{S^j_{\alpha\beta}} \left[\boldsymbol{t} - \rho^j_\alpha \widetilde{\boldsymbol{v}^j_\alpha} \left(\boldsymbol{v}^j_\alpha - \boldsymbol{w}^j_{\alpha\beta} \right) \right] \cdot d\boldsymbol{A} d\tau \tag{89}$$

General form of energy conservation equation

The general form of energy conservation equation for α phase within j sub-region can be derived according to Table 5 such that $\psi = E + 1/2v^2$, $i = \boldsymbol{t} \cdot \boldsymbol{v} + q$, $f = h + \boldsymbol{g} \cdot \boldsymbol{v}$ and $G = 0$ from Eq. (83):

$$\left(\overline{\rho^j_\alpha} \varepsilon^j_\alpha y^j \omega^j \right) \frac{\partial}{\partial t} \left(\overline{E + 1/2 v^{j\,2}_\alpha} \right) = \overline{\left(h^j_\alpha + \boldsymbol{g}^j_\alpha \cdot \boldsymbol{v}^j_\alpha \right) \rho^j_\alpha} \varepsilon^j_\alpha y^j \omega^j + \sum_{P=EXT,L,T,B,i}^{L=1\ldots N_K, i\neq j} I^{jP}_\alpha + \sum_{\beta\neq\alpha} I^j_{\alpha\beta} \tag{90}$$

where

$$I^{jP}_\alpha = \frac{1}{2\Delta t \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_S^{jP} \left[\boldsymbol{t} \cdot \boldsymbol{v}^j_\alpha + q - \rho^j_\alpha \overline{\left(E^j_\alpha + \left(v^j_\alpha \right)^2 / 2 \right)} \left(\boldsymbol{v}^j_\alpha - \boldsymbol{w}^{jP}_\alpha \right) \right] \cdot \gamma^j_a d\boldsymbol{A} d\tau$$

$$I^j_{\alpha\beta} = \frac{1}{2\Delta t \Sigma} \int_{t-\Delta t}^{t+\Delta t} \int_{S^j_{\alpha\beta}} \left[\boldsymbol{t} \cdot \boldsymbol{v}^j_\alpha - \rho^j_\alpha \overline{\left(E^j_\alpha + \left(v^j_\alpha \right)^2 / 2 \right)} \left(\boldsymbol{v}^j_\alpha - \boldsymbol{w}^j_{\alpha\beta} \right) \right] \cdot d\boldsymbol{A} d\tau,\ \beta \neq a$$

The l.h.s. term in Eq. (90) can be formulated as

$$\left(\overline{\rho^j_\alpha} \varepsilon^j_\alpha y^j \omega^j \right) \frac{\partial}{\partial t} \left(\overline{E + 1/2 v^{j2}_\alpha} \right)$$
$$= \left(\overline{\rho^j_\alpha} \varepsilon^j_\alpha y^j \omega^j \right) \frac{\partial}{\partial t} \left(\overline{E} + \frac{1}{2} \overline{v^j_\alpha v^j_\alpha} \right)$$

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$$= \left(\overline{\rho^j_\alpha \varepsilon^j_\alpha y^j \omega^j}\right) \frac{\partial}{\partial t} \left(\overline{E} + \overbrace{\frac{1}{2}\overline{\left(\widetilde{v^j_\alpha}\right)^2} + \frac{1}{2}\left(\overline{v^j_\alpha}\right)^2}^{\text{Lemma 1}} \right) \tag{91}$$

In the interest of brevity, we make the following definition.

Definition 19: The time averaged value of the generalized internal energy of B^j_α is defined as:

$$\widehat{E^j_\alpha} = \overline{E^j_\alpha} + \overline{\widetilde{v^j_\alpha}^2} \Big/ 2 \tag{92}$$

Definition 20: The fluctuation value of the generalized internal energy of B^j_α is defined as:

$$\overparen{E^j_\alpha} = E^j_\alpha - \widehat{E^j_\alpha} = \widetilde{E^j_\alpha} - \overline{\widetilde{v^j_\alpha}^2} \Big/ 2 \tag{93}$$

Definition 21: The time averaged value of the generalized external energy of B^j_α:

$$\widehat{h^j_\alpha} = \overline{h^j_\alpha} + \overline{\widetilde{\boldsymbol{g}^j_\alpha} \cdot \widetilde{\boldsymbol{v}^j_\alpha}} \tag{94}$$

Therefore, the l.h.s. term in Eq. (90) can be rewritten as

$$\left(\overline{\rho^j_\alpha \varepsilon^j_\alpha y^j \omega^j}\right) \frac{\partial}{\partial t} \left(\overline{E + 1/2 v^{j\,2}_\alpha}\right) = \left(\overline{\rho^j_\alpha \varepsilon^j_\alpha y^j \omega^j}\right) \frac{\partial}{\partial t} \left(\widehat{E} + \frac{1}{2}\left(\overline{v^j_\alpha}\right)^2 \right). \tag{95}$$

The first term on the r.h.s. can be formulated as

$$
\begin{aligned}
&\overline{\left(h^j_\alpha + \boldsymbol{g}^j_\alpha \cdot \boldsymbol{v}^j_\alpha\right)}\,\overline{\rho^j_\alpha}\varepsilon^j_\alpha y^j \omega^j \\
&= \left(\overline{h^j_\alpha} + \overline{\boldsymbol{g}^j_\alpha \cdot \boldsymbol{v}^j_\alpha}\right) \overline{\rho^j_\alpha}\varepsilon^j_\alpha y^j \omega^j \\
&= \left(\overline{h^j_\alpha} + \overbrace{\overline{\boldsymbol{g}^j_\alpha} \cdot \overline{\boldsymbol{v}^j_\alpha} + \overline{\widetilde{\boldsymbol{g}^j_\alpha} \cdot \widetilde{\boldsymbol{v}^j_\alpha}}}^{\text{Lemma 1}}\right) \overline{\rho^j_\alpha}\varepsilon^j_\alpha y^j \omega^j \\
&= \left(\widehat{h^j_\alpha} + \overline{\boldsymbol{g}^j_\alpha} \cdot \overline{\boldsymbol{v}^j_\alpha}\right) \overline{\rho^j_\alpha}\varepsilon^j_\alpha y^j \omega^j
\end{aligned}
\tag{96}
$$

The non-convective term across the interface S^{jP} can be formulated as

$$
\begin{aligned}
I^{jP}_\alpha &= \frac{1}{2\Delta t \Sigma}\int_{t-\Delta t}^{t+\Delta t}\int_{S}^{jP}\left[\boldsymbol{t}\cdot\boldsymbol{v}^j_\alpha + q - \rho^j_\alpha \overline{\left(E^j_\alpha + \left(v^j_\alpha\right)^2/2\right)}\left(\boldsymbol{v}^j_\alpha - \boldsymbol{w}^{jP}_\alpha\right)\right]\cdot\gamma^j_a d\boldsymbol{A}d\tau \\
&= \frac{1}{2\Delta t \Sigma}\int_{t-\Delta t}^{t+\Delta t}\int_{S^{jP}}\left[\boldsymbol{t}\cdot\left(\overline{\boldsymbol{v}^j_\alpha} + \widetilde{\boldsymbol{v}^j_\alpha}\right) + q - \rho^j_\alpha\left(\widetilde{E^j_\alpha} + \widetilde{\left(v^j_\alpha\right)^2}\Big/2\right)\left(\boldsymbol{v}^j_\alpha - \boldsymbol{w}^{jP}_\alpha\right)\right]\cdot\gamma^j_a d\boldsymbol{A}d\tau \\
&= \frac{1}{2\Delta t \Sigma}\int_{t-\Delta t}^{t+\Delta t}\int_{S^{jP}}\left[\boldsymbol{t}\cdot\overline{\boldsymbol{v}^j_\alpha} + \boldsymbol{t}\cdot\widetilde{\boldsymbol{v}^j_\alpha} + q - \rho^j_\alpha\left(\overbrace{\overline{\widetilde{E^j_\alpha}} + \overline{\widetilde{v^j_\alpha}^2}}^{\text{Definition 20}}\Big/2 + \overbrace{\frac{1}{2}\left(2\overline{v^j_\alpha}\widetilde{v^j_\alpha} + \widetilde{\widetilde{v^j_\alpha}^2}\right)}^{\text{Lemma 2}}\right)\left(\boldsymbol{v}^j_\alpha - \boldsymbol{w}^{jP}_\alpha\right)\right]\cdot\gamma^j_a d\boldsymbol{A}d\tau
\end{aligned}
$$

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$$= \frac{1}{2\Delta t \Sigma}\int_{t-\Delta t}^{t+\Delta t}\int_{S^{jP}} \left[\boldsymbol{t}\cdot\overline{\boldsymbol{v}^j_\alpha} + \boldsymbol{t}\cdot\widetilde{\boldsymbol{v}^j_\alpha} + q - \rho^j_\alpha \left(\overline{v^j_\alpha}\,\widetilde{v^j_\alpha} + \widehat{E^j_\alpha} + \frac{1}{2} \overbrace{\left(\overline{\widetilde{v^j_\alpha}^{2}} + \widetilde{v^j_\alpha}^{2}\right)}^{\text{Eq. (67)}}\right)\left(\boldsymbol{v}^j_\alpha - \boldsymbol{w}^{jP}_\alpha\right)\right]\cdot\gamma^j_a d\boldsymbol{A} d\tau$$

$$= \frac{1}{2\Delta t \Sigma}\int_{t-\Delta t}^{t+\Delta t}\int_{S^{jP}} \left[\boldsymbol{t}\cdot\overline{\boldsymbol{v}^j_\alpha} - \rho^j_\alpha \overline{v^j_\alpha}\,\widetilde{v^j_\alpha}\left(\boldsymbol{v}^j_\alpha - \boldsymbol{w}^{jP}_\alpha\right) + \boldsymbol{t}\cdot\widetilde{\boldsymbol{v}^j_\alpha} + q - \rho^j_\alpha \left(\widehat{E^j_\alpha} + \frac{1}{2}\widetilde{v^j_\alpha}^{2}\right)\left(\boldsymbol{v}^j_\alpha - \boldsymbol{w}^{jP}_\alpha\right)\right]\cdot\gamma^j_a d\boldsymbol{A} d\tau$$

$$= \left\{ \overbrace{\frac{1}{2\Delta t \Sigma}\int_{t-\Delta t}^{t+\Delta t}\int_{S^{jP}} \left[\boldsymbol{t} - \rho^j_\alpha \widetilde{v^j_\alpha}\left(\boldsymbol{v}^j_\alpha - \boldsymbol{w}^{jP}_\alpha\right)\right]\cdot\gamma^j_a d\boldsymbol{A} d\tau}^{\text{Eq. (88)}} \right\}\cdot\overline{\boldsymbol{v}^j_\alpha} +$$

$$\frac{1}{2\Delta t \Sigma}\int_{t-\Delta t}^{t+\Delta t}\int_{S^{jP}} \left[\boldsymbol{t}\cdot\widetilde{\boldsymbol{v}^j_\alpha} + q - \rho^j_\alpha \left(\widehat{E^j_\alpha} + \frac{1}{2}\widetilde{v^j_\alpha}^{2}\right)\left(\boldsymbol{v}^j_\alpha - \boldsymbol{w}^{jP}_\alpha\right)\right]\cdot\gamma^j_a d\boldsymbol{A} d\tau$$

In the interest of brevity, we make the definition of generalized energy exchange term across the interface S^{jP} as

$$Q_\alpha^{jP} = \frac{1}{2\Delta t\Sigma}\int_{t-\Delta t}^{t+\Delta t}\int_{S^{jP}}\left[q + \boldsymbol{t}\cdot\widetilde{\boldsymbol{v}_\alpha^j} - \rho_\alpha^j\left(\widehat{E_\alpha^j} + \frac{1}{2}\widetilde{v_\alpha^j}^2\right)\left(\boldsymbol{v}_\alpha^j - \boldsymbol{w}_\alpha^{jP}\right)\right]\cdot\gamma_a^j d\boldsymbol{A}d\tau . \tag{97}$$

Therefore, the non-convective term across interface S^{jP} can be rewritten as

$$I_\alpha^{jP} = \boldsymbol{T}_\alpha^{jP}\cdot\overline{\boldsymbol{v}_\alpha^j} + Q_\alpha^{jP} \tag{98}$$

Similarly, the non-convective term across the interface $S_{a\beta}^j$ can be rewritten as

$$I_{\alpha\beta}^j = \boldsymbol{T}_{\alpha\beta}^j\cdot\overline{\boldsymbol{v}_\alpha^j} + Q_{\alpha\beta}^j \tag{99}$$

where $Q_{\alpha\beta}^j$ is the generalized energy exchange term across the interface $S_{a\beta}^j$, and

$$Q_{\alpha\beta}^j = \frac{1}{2\Delta t\Sigma}\int_{t-\Delta t}^{t+\Delta t}\int_{S_{\alpha\beta}^j}\left[q + \boldsymbol{t}\cdot\widetilde{\boldsymbol{v}_\alpha^j} - \rho_\alpha^j\left(\widehat{E_\alpha^j} + \frac{1}{2}\widetilde{v_\alpha^j}^2\right)\left(\boldsymbol{v}_\alpha^j - \boldsymbol{w}_{\alpha\beta}^j\right)\right]\cdot d\boldsymbol{A}d\tau \tag{100}$$

Substitution of Eq. (95), Eq. (96), Eq. (98), and Eq. (99) into Eq. (90) yields the general form of averaged energy conservation equation.

$$\left(\overline{\rho_\alpha^j}\varepsilon_\alpha^j y^j\omega^j\right)\frac{d}{dt}\left(\widehat{E_\alpha^j} + \overline{v_\alpha^j}^2\Big/2\right)$$
$$= \left(\widehat{h_\alpha^j} + \overline{\boldsymbol{g}_\alpha^j}\cdot\overline{\boldsymbol{v}_\alpha^j}\right)\overline{\rho_\alpha^j}\varepsilon_\alpha^j y^j\omega^j + \sum_{P=EXT,L,T,B,i}^{L=1\ldots N_K, i\neq j}\left(\boldsymbol{T}_\alpha^{jP}\cdot\overline{\boldsymbol{v}_\alpha^j} + Q_\alpha^{jP}\right) + \sum_{\beta\neq\alpha}\left(\boldsymbol{T}_{\alpha\beta}^j\cdot\overline{\boldsymbol{v}_\alpha^j} + Q_{\alpha\beta}^j\right). \tag{101}$$

After dot product of the velocity vector $\overline{\boldsymbol{v}_\alpha^j}$ with the momentum balance Eq. (87) we will get the mechanical energy conservation equation:

$$\left(\overline{\rho_\alpha^j}\varepsilon_\alpha^j y^j \omega^j\right)\frac{d}{dt}\left(\overline{v_\alpha^j}^2\Big/2\right)$$

$$=\overline{\boldsymbol{g}_\alpha^j}\cdot\overline{\boldsymbol{v}_\alpha^j\rho_\alpha^j}\varepsilon_\alpha^j y^j\omega^j+\sum_{P=EXT,L,T,B,i}^{L=1\ldots N_K,i\neq j}\left(\boldsymbol{T}_\alpha^{jP}\cdot\overline{\boldsymbol{v}_\alpha^j}\right)+\sum_{\beta\neq\alpha}\left(\boldsymbol{T}_{\alpha\beta}^j\cdot\overline{\boldsymbol{v}_\alpha^j}\right). \tag{102}$$

And the internal energy conservation equation is obtained from Eq. (101), after subtraction of the mechanical energy conservation Eq. (102):

$$\left(\overline{\rho_\alpha^j}\varepsilon_\alpha^j y^j\omega^j\right)\frac{d\widehat{E_\alpha^j}}{dt}=\widehat{h_\alpha^j}\overline{\rho_\alpha^j}\varepsilon_\alpha^j y^j\omega^j+\sum_{P=EXT,L,T,B,i}^{L=1\ldots N_K,i\neq j}Q_\alpha^{jP}+\sum_{\beta\neq\alpha}Q_{\alpha\beta}^j. \tag{103}$$

Furthermore, after ignoring any additional item caused by the fluctuation of velocity and internal energy in Eq. (103), the balance equation of heat is derived:

$$\left(\varepsilon_\alpha^j y^j\omega^j c_\alpha^j\right)\frac{d\overline{\theta_\alpha^j}}{dt}=\overline{h_\alpha^j\rho_\alpha^j}\varepsilon_\alpha^j y^j\omega^j+\sum_{P=EXT,L,T,B,i}^{L=1\ldots N_K,i\neq j}\widehat{Q_\alpha^{jP}}+\sum_{\beta\neq\alpha}\widehat{Q_{\alpha\beta}^j}, \tag{104}$$

where c_α^j represents the specific heat capacity of α phase at constant volume averaged over j zone, $\overline{\theta_a^j}$ represents the temperature of α phase averaged over j zone, $\widehat{Q_\alpha^{jP}}$ represents the heat transferred from α phase in P zone to that in j zone, $\widehat{Q_{\alpha\beta}^j}$ represents the heat transferred from β phase to α phase in j zone, and

$$\widehat{Q_\alpha^{jP}}=\frac{1}{2\Delta t\Sigma}\int_{t-\Delta t}^{t+\Delta t}\int_{S^{jP}}q\cdot\gamma_a^j d\boldsymbol{A}d\tau \tag{105}$$

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$$\widehat{Q^j_{\alpha\beta}} = \frac{1}{2\Delta t\Sigma}\int_{t-\Delta t}^{t+\Delta t}\int_{S^j_{\alpha\beta}} q\cdot d\boldsymbol{A}d\tau \tag{106}$$

For convenience, $\widehat{Q^{jP}_\alpha}$ and $\widehat{Q^j_{\alpha\beta}}$ are still denoted by Q^{jP}_α and $Q^j_{\alpha\beta}$ unless otherwise confusion arises. The final result of heat balance equation is as following:

$$\left(\varepsilon^j_\alpha y^j \omega^j c^j_\alpha\right)\frac{d\overline{\theta^j_\alpha}}{dt} = \overline{h^j_\alpha \rho^j_\alpha}\varepsilon^j_\alpha y^j \omega^j + \sum_{P=EXT,L,T,B,i}^{L=1\ldots N_K,i\neq j} Q^{jP}_\alpha + \sum_{\beta\neq\alpha} Q^j_{\alpha\beta} \tag{107}$$

General form of entropy conservation equation

The general form of the entropy conservation equation for α phase within j sub-region can be derived according to Table 5 such that $\psi=\eta$, $i=j$, $f=b$ and $G=L$ from Eq. (86) (for clarity, non-convective entropy is denoted by the symbol F):

$$\left(\overline{\rho^j_\alpha}\varepsilon^j_\alpha y^j \omega^j\right)\frac{d\overline{\eta^j_\alpha}}{dt} = \overline{b^j_\alpha \rho^j_\alpha}\varepsilon^j_\alpha y^j \omega^j + \overline{L^j_\alpha}\varepsilon^j_\alpha y^j \omega^j + \sum_{P=EXT,L,T,B,i}^{L=1\ldots N_K,i\neq j} F^{jP}_\alpha + \sum_{\beta\neq\alpha} F^j_{\alpha\beta} \tag{108}$$

where:

$$F^{jP}_\alpha = \frac{1}{2\Delta t\Sigma}\int_{t-\Delta t}^{t+\Delta t}\int_{S^{jP}} \left[j - \rho^j_\alpha \widetilde{\eta^j_\alpha}\left(\boldsymbol{v}^j_\alpha - \boldsymbol{w}^{jP}_\alpha\right)\right]\cdot \gamma^j_a d\boldsymbol{A}d\tau$$
$$P = EXT, L, T, B, i, L = 1\ldots N_K, i\neq j \tag{109}$$

$$F^j_{\alpha\beta} = \frac{1}{2\Delta t\Sigma}\int_{t-\Delta t}^{t+\Delta t}\int_{S^j_{\alpha\beta}} \left[j - \rho^j_\alpha \widetilde{\eta^j_\alpha}\left(\boldsymbol{v}^j_\alpha - \boldsymbol{w}^j_{\alpha\beta}\right)\right]\cdot d\boldsymbol{A}d\tau, \beta\neq\alpha \tag{110}$$

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Nomenclature

Latin symbols

b	the entropy supply from the external world	
B	the body of a continuum	
$B(K)$	the K th REW	
$B^j(K)$	the body of j sub-region continuum divided from $B(K)$, $j \in \{e \mid e = u, s, r, t, b, v, n, g\}$	
$B^j_\alpha(K)$	the body of α phase in j sub-region divided from $B(K)$, $j \in \{e \mid e{=}u, s, r, t, b, v, n, g\}$, $\alpha \in \{\zeta \mid \zeta = m, l, a, p, i, n, v\}$	
c^j	the specific heat capacity of j zone at a constant volume	$\left[L^2T^{-2}\Theta^{-1}\right]$
c^j_α	the specific heat capacity of α phase in j zone at a constant volume	$\left[L^2T^{-2}\right]$
$C(K)$	the contour of $S^{,T}(K)$	
$d\mathbf{S}^{jEXT}(K)$	the differential area vector for $S^{jEXT}(K)$	$\left[L^2\right]$
$d\mathbf{S}^{jL}(K)$	the differential area vector for $S^{jL}(K)$	$\left[L^2\right]$
$d\mathbf{S}^{jT}(K)$	the differential area vector for $S^{jT}(K)$	$\left[L^2\right]$
$d\mathbf{S}^{jB}(K)$	the differential area vector for $S^{jB}(K)$	$\left[L^2\right]$
$d\mathbf{S}^{ji}(K)$	the differential area vector for $S^{ji}(K)$	$\left[L^2\right]$
$d\mathbf{S}^j_{\alpha\beta}(K)$	the differential area vector for $S^j_{\alpha\beta}(K)$	$\left[L^2\right]$
e^{jP}_α	the net flux of α phase through S^{jP}	$ML^{-2}T^{-1}$
$e^j_{\alpha\beta}$	the phase transition rate between α phase and β phase	$ML^{-2}T^{-1}$
E	the microscopic internal energy per unit mass	$\left[L^2T^{-2}\right]$

$\widehat{E_\alpha^j}$	the time-averaged value of the generalized internal energy of B_α^j	$[MT^{-2}]$
$\widetilde{E_\alpha^j}$	the fluctuation value of the generalized internal energy of B_α^j	$[MT^{-2}]$
f	the source or sink term per unit mass	
$\overline{f_\alpha^j}$	the time-averaged generation rate of α phase in j zone per unit mass	
$\boldsymbol{g}$	the gravity accelerator vector	$[LT^{-2}]$
G	the source or sink term per unit volume	
$\overline{G_\alpha^j}$	the time-averaged generation rate of α phase in j zone per unit volume	
h	the supply of internal energy from outside world	$[MT^{-3}]$
$\widehat{h_\alpha^j}$	the time-averaged value of the generalized external energy of B_α^j	$[MT^{-3}]$
$\boldsymbol{i}$	the diffusion flux	
I_α^{jP}	the non-convective term of physical quantity $\boldsymbol{\phi}$ through the interface S_α^{jP}	
$I_{\alpha\beta}^j$	the non-convective term of physical quantity $\boldsymbol{\phi}$ through the interface $S_{\alpha\beta}^j$	
$\boldsymbol{j}$	the non-convective flux of entropy	
K	indicate the K th REW	
L	the entropy production within the continuum	
m^r	the time-averaged cross section area of the main channel reach	$[L^2]$
M	the number of discrete REWs in a watershed	

N_K	the number of REWs neighboring $B(K)$	
$P^o(K)$	the nadir of $C(K)$, watershed outlet	
$\boldsymbol{q}$	the microscopic heat flux vector	$\left[MT^{-3}\right]$
Q_α^{jP}	the generalized energy exchange term across the interface S^{jP}	$\left[MT^{-3}\right]$
$Q_{\alpha\beta}^j$	the generalized energy exchange term across the interface $S_{\alpha\beta}^j$	$\left[MT^{-3}\right]$
$\widehat{Q_\alpha^{jP}}$	the heat transferred from α phase in P zone to that in j zone	$\left[MT^{-3}\right]$
$\widehat{Q_{\alpha\beta}^j}$	the heat transferred from β phase to α phase in j zone	$\left[MT^{-3}\right]$
R_n	the intensity of radiation	$\left[MT^{-3}\right]$
$S(K)$	the surface of $B(K)$	$\left[L^2\right]$
$S^{,EXT}(K)$	the segment formed by the interfaces between $B(K)$ and the external world	$\left[L^2\right]$
$S^{,L}(K)$	the segment formed by the interfaces between $B(K)$ and $B(L)$	$\left[L^2\right]$
$S^{,T}(K)$	the top surface formed by the land surface covering $B(K)$	$\left[L^2\right]$
$S^{,B}(K)$	the bottom surface of $B(K)$, can be either the impermeable strata or a hypothetical plane at a given depth reaching into the groundwater reservoir, or a combination of the two	$\left[L^2\right]$
$S^{jEXT}(K)$	the interface between $B^j(K)$ and the external world	$\left[L^2\right]$
$S^{jL}(K)$	the interface between $B^j(K)$ and $B(L)$ $(L=1..N_K)$	$\left[L^2\right]$
$S^{jT}(K)$	the interface between $B^j(K)$ and the atmosphere	$\left[L^2\right]$

$S^{jB}(K)$	the interface between $B^j(K)$ and the impermeable strata or the groundwater reservoir	$[L^2]$
$S^{ji}(K)$	the interface between $B^j(K)$ and other sub-regions within the same REW, $B^i(K)\,(i \neq j)$	$[L^2]$
$S^j_{\alpha\beta}(K)$	the phase interface between $B^j_\alpha(K)$ and $B^j_\beta(K)$	$[L^2]$
$\boldsymbol{S}^{jP}(K)$	the area vector of interface $S^{jP}(K)$	$[L^2]$
$\boldsymbol{t}$	the microscopic stress tensor	$[ML^{-1}T^{-2}]$
$\boldsymbol{T}^{jP}_\alpha$	the non-convective momentum through the interface S^{jP}_α	$[MLT^{-2}]$
$\boldsymbol{v}$	velocity of the a continuum	$[LT^{-1}]$
$V(K)$	the space occupied by all the substances contained in $B(K)$	$[L^3]$
$V^j(K)$	the volume occupied by $B^j(K)$	$[L^3]$
$V^j_\alpha(K)$	the volume occupied by $B^j_\alpha(K)$	$[L^3]$
$\boldsymbol{w}$	velocity of a continuum interface	$[LT^{-1}]$
y^j	the time-averaged thickness of B^j	$[L]$

Greek symbols

Δt	time interval for equation averaging	$[T]$
ε^j_α	the time-averaged volume of B^j_α relative to V^j	
ε^u_l	water content of the unsaturated zone	
ε^s_l	water content of the saturated zone	
$\boldsymbol{\phi}$	physical quantity	

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γ_α^j	the phase distribution function on α phase in j zone	
η	the microscopic entropy per unit mass	
κ_α^{jP}	the fraction of heat exchange term Q^{jP} absorbed by α phase	
λ_α	the fraction of fusion heat absorbed by α phase	
$\overline{\theta^{surf}}$	the averaged temperature of the surface sub-regions	$[\Theta]$
$\underline{\theta_\alpha^j}$	the temperature of α phase in j zone	$[\Theta]$
$\overline{\rho_\alpha^j}$	the time-averaged density of B_α^j	$\left[ML^{-3}\right]$
ρ_α^j	the density of α phase at the differential volume dV in V_α^j space	$\left[ML^{-3}\right]$
$\Sigma(K)$	the horizontal projected area of $B(K)$	$\left[L^2\right]$
$\Sigma^j(K)$	the horizontal projected area of $B^j(K)$	$\left[L^2\right]$
ω^j	the time-averaged horizontal projected area of B^j	$\left[L^2\right]$
ξ^r	the time-averaged length of the main channel reach relative to Σ	$[L]$
ψ_α^j	the instantaneous value of physical quantity $\boldsymbol{\phi}$ possessed by B_α^j relative to the mass of B_α^j	
$\overline{\psi_\alpha^j}$	the time-averaged physical quantity $\boldsymbol{\phi}$ possessed by B_α^j relative to the mass of B_α^j	
$\widetilde{\psi_\alpha^j}$	the fluctuant value of physical quantity $\boldsymbol{\phi}$ possessed by B_α^j relative to the mass of B_α^j	

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Subscripts and superscripts

B	superscript indicating the impermeable strata or groundwater reservoir
EXT	superscript indicating the external world
i, j	superscripts indicating sub-region, can be u (unsaturated zone), s(saturated zone), r (main channel reach), t (sub-stream network), b (bared soil zone), v (vegetation covered zone), n (snow covered zone), g (glacier covered zone)
L	superscript indicating the neighboring REW, $L=1..N_K$
P	superscript indicating the wildcard indicating $EXT, L, T, B, i, L=1..N_K$
T	superscript indicating the atmosphere
α, β	subscripts indicating the phase, can be m (soil matrix), l (liquid water), a (gaseous phase), p (vapor), i (ice), n (snow), and v (vegetation)

Note: M is the dimension of mass, L is the dimension of length, T is the dimension of time, and Θ is the dimension of temperature.

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References

Abbott, M. B., Bathurst, J. C., Cunge, J. A., O'Connell, P. E., and Rasmussen, J.: An introduction to the European Hydrological System – Systeme Hydrologique European, SHE, 1: History and philosophy of a physically based, distributed modeling system, J. Hydrol., 87, 45–59, 1986a.

Abbott, M. B., Bathurst, J. C., Cunge, J. A., O'Connell, P. E., and Rasmussen, J.: An introduction to the European Hydrological System – Systeme Hydrologique European, SHE, 2: Structure of a physically based, distributed modeling system, J. Hydrol., 87, 61–77, 1986b.

Adrie, F. G. J., Bert, G. H., and Simon, M. B.: Dew deposition and drying in a desert system: A simple simulation model, J. Arid Environ., 42, 211–222, 1999.

Arnold, J., Srinivasan, G. R., Muttiah, R. S., and Williams, J. R.: Large area hydrologic modeling and assessment, part I: Model development, J. Amer. Water Res. Assoc., 34, 73–89, 1998.

Beven, K. J., Calver, A., and Morris, E.: The Institute of Hydrology distributed model, Institute of Hydrology Report No. 98, UK, 1987.

Beven, K. J.: Changing ideas in hydrology-the case of physically-based models, J. Hydrol., 105, 157–172, 1989.

Beven, K. J.: Prophecy, reality and uncertainty in distributed hydrological modeling, Adv. Water Resour., 16, 41–51, 1993.

Beven, K. J.: A discussion of distributed modelling, in: Distributed Hydrological Modelling, edited by: Refsgaard, J. C. and Abbott, M. B., Kluwer, Dordrecht, Netherlands, 255–278, 1996.

Beven, K. J.: Towards an alternative blueprint for a physically based digitally simulated hydrologic response modelling system, Hydrol. Process., 16, 189–206, 2002.

Calver, A. and Wood, W. L.: The Institute of Hydrology distributed model, in: Computer models

of watershed hydrology, edited by: Singh, V. P., Water Resources Publications, USA, 595–626, 1995.
Dunne, T., Moore, T. R., and Taylor, C. H.: Recognition and prediction of runoff-producing zones in humid regions, Hydrol. Sci. J., 20(3), 305–327, 1975.
Dunne, T.: Field studies of hillslope flow processes, in: Hillslope Hydrology, edited by Kirkby, M. J., John Wiley & Sons, Chichester, UK, 227–293, 1978.
Freeze, R. A., Harlan, R. L.: Blueprint for a physically-based digitally-simulated hydrological response model, J. Hydrol., 9, 237–258, 1969.
Grayson, R. B., Moore, I. D., and McMahon, T. A.: Physically-based hydrologic modeling: 2. Is the concept realistic, Water Resour. Res., 28, 2659–2666 , 1992.
Hassanizadeh, S. M. and Gray, W. G.: General conservation equations for multiphase systems: 1. Averaging procedure, Adv. Water Resour., 2, 131–144, 1979a.
Hassanizadeh, S. M. and Gray, W. G.: General conservation equations for multiphase systems: 2. Mass, momenta, energy and entropy equations, Adv. Water Resour., 2, 191–203, 1979b.
Hassanizadeh, S. M. and Gray, W. G.: General conservation equations for multiphase systems, 3. Constitutive theory for porous media flow, Adv. Water Resour., 3, 25–40, 1980.
Hassanizadeh, S. M.: Derivation of basic equations of mass transport in porous media, part 1: Macroscopic balance laws, Adv. Water Resour., 9, 196–206, 1986a.
Hassanizadeh, S. M.: Derivation of basic equations of mass transport in porous media, part 2: Generalized Darcy's law and Fick's law, Adv. Water Resour., 9, 207–222, 1986b.
Lee, H., Sivapalan, M., and Zehe, E.: Representative Elementary Watershed (REW) approach, a new blueprint for distributed hydrologic modelling at the catchment scale, Ch. 15, in: Predictions in Ungauged Basins: International Perspectives on State-of-the-Art and Pathways Forward, edited by Franks, S. W., Sivapalan, M., Takeuchi, K., and Tachikawa, Y., IAHS Press, Wallingford, Oxon, UK, in press, 2005a.
Lee, H., Sivapalan, M., and Zehe, E.: Representative Elementary Watershed (REW) approach, a new blueprint for distributed hydrologic modelling at the catchment scale: the development of closure relations, in: Predicting Ungauged Streamflows in the Mackenzie River Basin: Today's Techniques and Tomorrow's Solutions, edited by Spence, C., Pomeroy, J. W., and Pietroniro, A., Canadian Water Resources Association (CWRA), Ottawa, Canada, 165–218, 2005b.
Lee, H., Sivapalan, M., and Zehe, E.: Representative Elementary Watershed (REW) approach, a new blueprint for distributed hydrologic modelling at the catchment scale: Numerical imple-

mentation, in: Physically Based Models of River Runoff and Their Application to Ungauged Basins, Proceedings, NATO Advanced Research Workshop, edited by O'Connell, P. E. and Kuchment, L., Newcastle-upon-Tyne, UK, in press, 2005c.
Refsgaard, J. C. and Storm, B.: MIKE SHE, in: Computer Models of Watershed Hydrology, edited by: Singh, V. P., Water Resources Publications, USA, 809–846, 1995.
Refsgaard, J. C., Storm, B. and Abbott, M. B.: Comment on "A discussion of distributed hydrological modelling" by Beven, K. J., in: Distributed Hydrological Modelling, edited by: Refsgaard, J. C. and Abbott, M. B., Kluwer, Dordrecht, Netherlands, 279–287, 1996.
Reggiani, P., Sivapalan, M., and Hassanizadeh, S. M.: A unifying framework for watershed thermodynamics: balance equations for mass, momentum, energy and entropy, and the second law of thermodynamics. Adv. Water Resour., 22(4), 367–398, 1998.
Reggiani, P., Hassanizadeh, S. M., and Sivapalan, M.: A unifying framework for watershed thermodynamics: constitutive relationships, Adv. Water Resour., 23, 15–39, 1999.
Reggiani, P. and Sivapalan, M.: Conservation equations governing hillslope responses: Exploring the physical basis of water balance, Water Resour. Res., 36, 1845–1863, 2000.
Reggiani, P., Sivapalan, M., Hassanizadeh, S. M., and Gray, W. G.: Coupled equations for mass and momentum balance in a stream network: theoretical derivation and computational experiments, Proc. R. Soc. Lond., Series A, 457, 157–189, 2001.
Reggiani, P. and Rientjes, T. H. M.: Flux parameterization in the representative elementary watershed approach: application to a natural basin, Water Resour. Res., 41, 1–18, 2005.
Robinson, J. S. and Sivapalan, M.: Catchment-scale runoff generation model by aggregation and similarity analyses, Hydrol. Process., 9, 555–574, 1995.
Rodriguez-Iturbe, I. and Rinaldo, A.: Fractal River Basins: Chance and Self-organization, Cambridge University Press, New York, USA, 1997.
Rui X. F.: Principles of Hydrology, China Water Power Press, Beijing, China, 143–152, 2004.
Singh, V. P. and Woolhiser, D. A.: Mathematical modeling of watershed hydrology, J. Hydraul. Eng., 7, 270–292, 2002.
Smith, R. E., Goodrich, D. R., Woolhiser, D. A., and Simanton, J. R.: Comments on "Physically-based hydrologic modelling: 2. Is the concept realistic?" by Grayson, R. B., Moore, I. D., and McMahon, T. A., Water Resour. Res., 30, 851–854, 1994.
Srinivasan, R., Ramanarayanan, T. S., Arnold, J. G., and Bednarz, S. T.: Large area hydrologic modeling and assessment, part II: Model application, J. Amer. Water Resour. Assoc., 34, 91–101, 1998.

Viney, N. R. and Sivapalan, M.: A framework for scaling of hydrologic conceptualisations based on a disaggregation-aggregation approach, Hydrol. Process., 18, 1395–1408, 2004.

Whitaker, S.: Introduction to Fluid Mechanics, Krieger, Malabar, Florida, 1981.

Woolhiser, D. A.: Search for physically-based runoff model – a hydrologic El Dorado, J. Hydraul. Eng., ASCE, 122, 122–129, 1996.

Yang, D., Herath, S., and Musiake, K.: Comparison of different distributed hydrological models for characterization of catchment spatial variability, Hydrol. Process., 14, 403–416, 2000.

Yang, D., Herath, S., and Musiake, K.: Hillslope-based hydrological model using catchment area and width functions, Hydrol. Sci. J., 47(1), 49–65, 2002a.

Yang, D., Oki, T., Herath, S., and Musiake, S.: A geomorphology-based hydrological model and its applications, in: Mathematical Models of Small Watershed Hydrology and Applications, edited by: Singh, V. P. and Frevert, D. K., Water Resources Publications, Littleton, Colorado, Chapter 9, 259–300, 2002b.

Zhang G. P. and Savenije, H. H. G.: Rainfall-runoff modeling in a catchment with a complex groundwater flow system: application of the Representative Elementary Watershed (REW) approach, Hydrol. Earth Syst. Sci., 9, 243–261, 2005.

Table 1. Sub-regions and materials of a REW after Reggiani (1998).

No.	sub-region	materials contained
1	saturated zone	water, soil matrix
2	unsaturated zone	water, gas, soil matrix
3	saturated overland flow zone	water
4	concentrated overland flow zone	water
5	main channel reach	water

Table 2. Structure of redefined REW (sub-regions).

No.	layer	sub-region	abbreviation
1	subsurface	**u**nsaturated zone	u
2	subsurface	**s**aturated zone	s
3	surface	main channel **r**each zone	r
4	surface	sub s**t**ream network zone	t
5	surface	**b**ared zone	b
6	surface	**v**egetation covered zone	v
7	surface	s**n**ow covered zone	n
8	surface	**g**lacier covered zone	g

Table 3. Materials contained in each sub-region.

No.	sub-region	materials	abbreviation
1	u-zone	soil **m**atrix	m
2	u-zone	**l**iquid water	l
3	u-zone	g**a**s	a
4	u-zone	**i**ce	i
5	s-zone	soil **m**atrix	m
6	s-zone	**l**iquid water	l
7	s-zone	**i**ce	i
8	r-zone	**l**iquid water	l
9	r-zone	va**p**or	p
10	t-zone	**l**iquid water	l
11	t-zone	va**p**or	p
12	b-zone	soil **m**atrix	m
13	b-zone	**l**iquid water	l
14	b-zone	va**p**or	p
15	v-zone	**v**egetation	v
16	v-zone	**l**iquid water	l
17	v-zone	va**p**or	p
18	n-zone	s**n**ow	n
19	n-zone	**l**iquid water	l
20	n-zone	g**a**s	a
21	g-zone	**i**ce	i
22	g-zone	**l**iquid water	l
23	g-zone	va**p**or	p

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Table 4. All materials involved in REW.

No.	materials	abbreviation
1	soil **m**atrix	m
2	**l**iquid water	l
3	g**a**s	a
4	va**p**or	p
5	**i**ce	i
6	s**n**ow	n
7	**v**egetation	v

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Table 5. Summary of the properties in the conservation equation (after Reggiani, 1998).

Quantity	ψ	i	f	G
Mass	1	0	0	0
Linear Momentum	$\boldsymbol{v}$	$\boldsymbol{t}$	$\boldsymbol{g}$	0
Energy	$E+1/2v^2$	$\boldsymbol{t}\cdot\boldsymbol{v}+\boldsymbol{q}$	$h+\boldsymbol{g}\cdot\boldsymbol{v}$	0
Entropy	η	$\boldsymbol{j}$	b	L

Note: Where, $\boldsymbol{t}$ is the microscopic stress tensor, $\boldsymbol{g}$ is the gravity acceleration vector, E is the microscopic internal energy per unit mass, $\boldsymbol{q}$ is the microscopic heat flux vector, h is the supply of internal energy from outside world, η is the microscopic entropy per unit mass, $\boldsymbol{j}$ is the non-convective flux of entropy, b is the entropy supply from the external world, L is the entropy production within the continuum.

Table 6. Summary of the interfaces for each sub-region.

No	Sub-region	Interfaces
1	s -zone	$S^{sB}, S^{sEXT}, S^{sL}, S^{su}, S^{sr}, S^{st}, S^{s}_{li}$
2	u-zone	$S^{us}, S^{uEXT}, S^{uL}, S^{ub}, S^{uv}, S^{ug}, S^{un}, S^{u}_{li}$
3	b-zone	$S^{bT}, S^{br}, S^{bu}, S^{b}_{lp}$
4	v-zone	$S^{vT}, S^{vr}, S^{vu}, S^{v}_{lp}$
5	n-zone	$S^{nT}, S^{nr}, S^{nu}, S^{n}_{lp}$
6	g-zone	$S^{gT}, S^{gr}, S^{gu}, S^{g}_{lp}$
7	r-zone	$S^{rT}, S^{rEXT}, S^{rL}, S^{rt}, S^{rs}, S^{r}_{lp}$
8	t-zone	$S^{tT}, S^{tb}, S^{tv}, S^{tn}, S^{tg}, S^{tr}, S^{ts}, S^{t}_{lp}$

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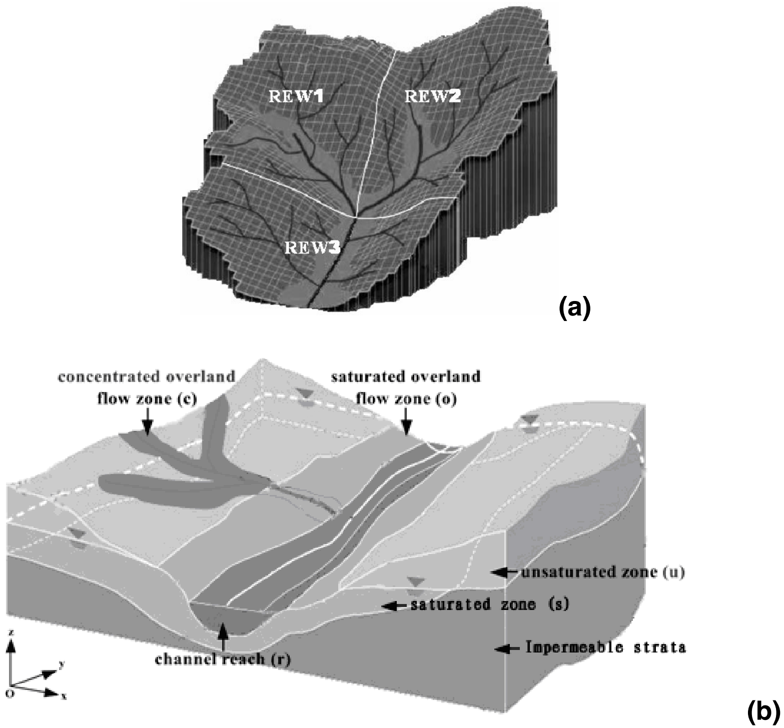

Fig. 1. **(a)** Catchment discretization into 3 REW units **(b)** Sub-regions making up the spatial domain of a REW (after Reggiani et al., 1998 and Lee et al., 2005).

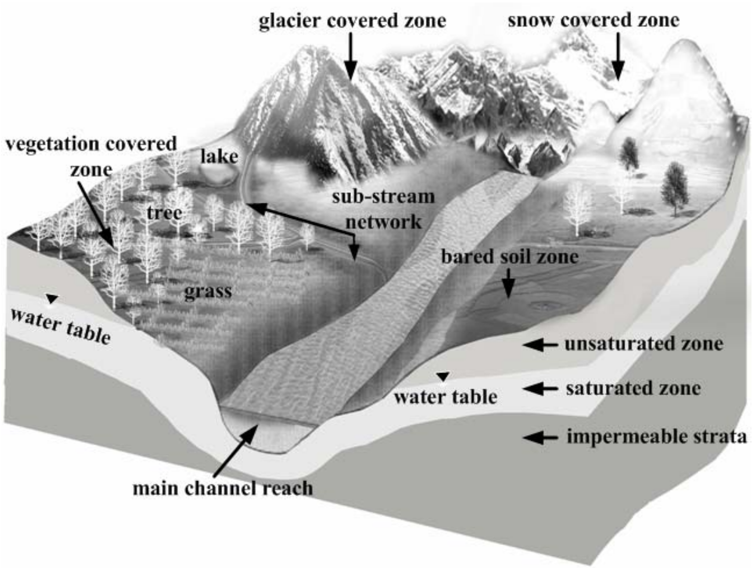

Fig. 2. Sub-regions of the redefined REW.